


1663

Climate labs built to travel
Precision tumor targeting
Magnetically expanded metal
Portable particle accelerator
COVID-19: Los Alamos fights back

NOT MICROPLASTICS, MICROBEPLASTICS



Diamond-nanocrystal pyramids—millionths of a meter wide at the base and just billionths of a meter at the tip—serve as high-precision electron emitters for a new kind of tabletop particle accelerator. While such an accelerator would not produce particles nearly as energetic as those from high-energy-physics research facilities, it would nonetheless make practical, portable particle beams for a tremendous variety of important medical, scientific, and national security applications. To learn more about the emitters (seen here through a scanning electron microscope) and other components Los Alamos scientists are fabricating to make this new technology possible, see “The Tabletop Beam Machine” on page 34.

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LOS ALAMOS SCIENCE AND
TECHNOLOGY MAGAZINE

ABOUT THE COVER

Microorganisms, such as bacteria, fungi, and algae, are the tiny workhorses of the planet. Bacteria and fungi decompose organic matter into nutrients consumed by plants, and algae release vital oxygen into the atmosphere while they are busy making their own food from sunlight and carbon dioxide. But get this: the molecules that microbes are making during these various processes resemble the building blocks of plastics—so, what if microbes could be tasked with making plastics? And what if these plastics were better than existing ones? Instead of breaking down into smaller and smaller pieces of garbage—microplastics—that pollute our oceans and contaminate water and food sources, perhaps they could break down into something more useful. Los Alamos scientists are among a growing community of researchers developing microbes that can make such new plastics possible. And if they succeed, then *micro*beplastics could make microplastics a thing of the past.

ABOUT OUR NAME

During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

ABOUT THE LDRD LOGO

Laboratory Directed Research and Development (LDRD) is a competitive internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to national interests. Whenever *1663* reports on research that received support from LDRD, this logo appears at the end of the article.

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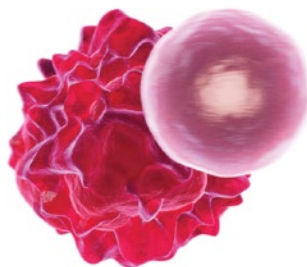


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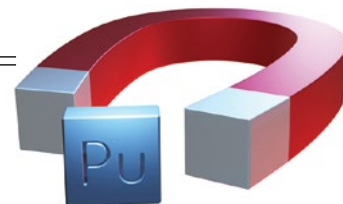
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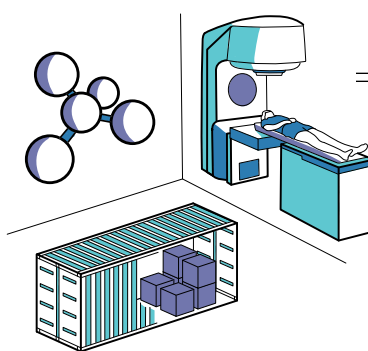
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INFECTIOUS DISEASE

Los Alamos
Versus the Virus

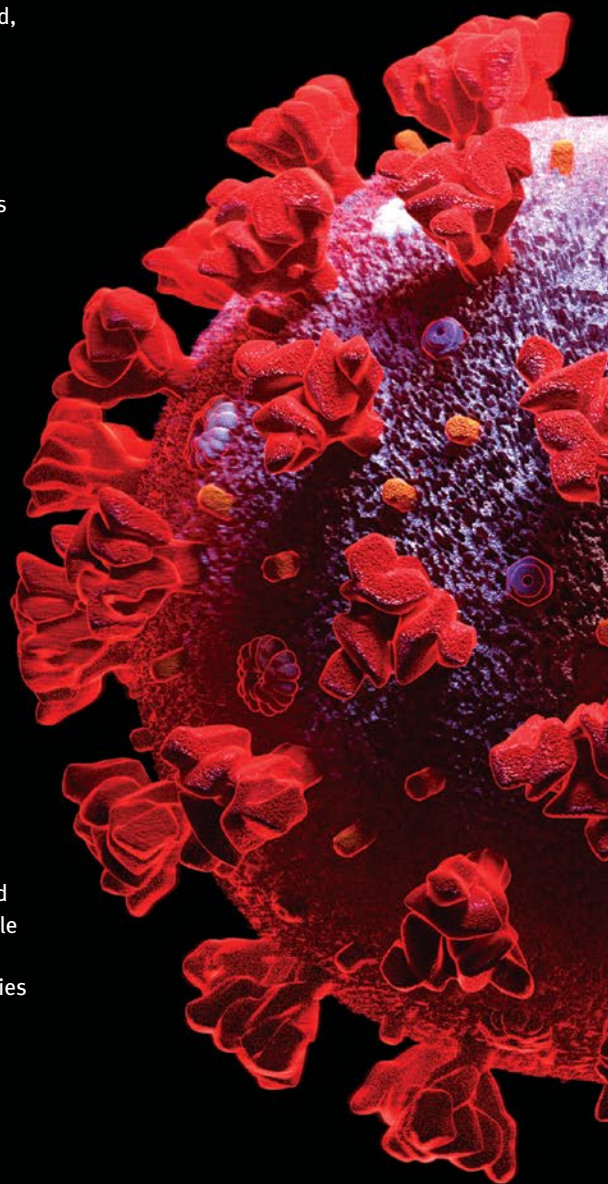
Los Alamos responded to the COVID-19 threat with rigorous worker isolation and a massive mobilization of scientific resources.

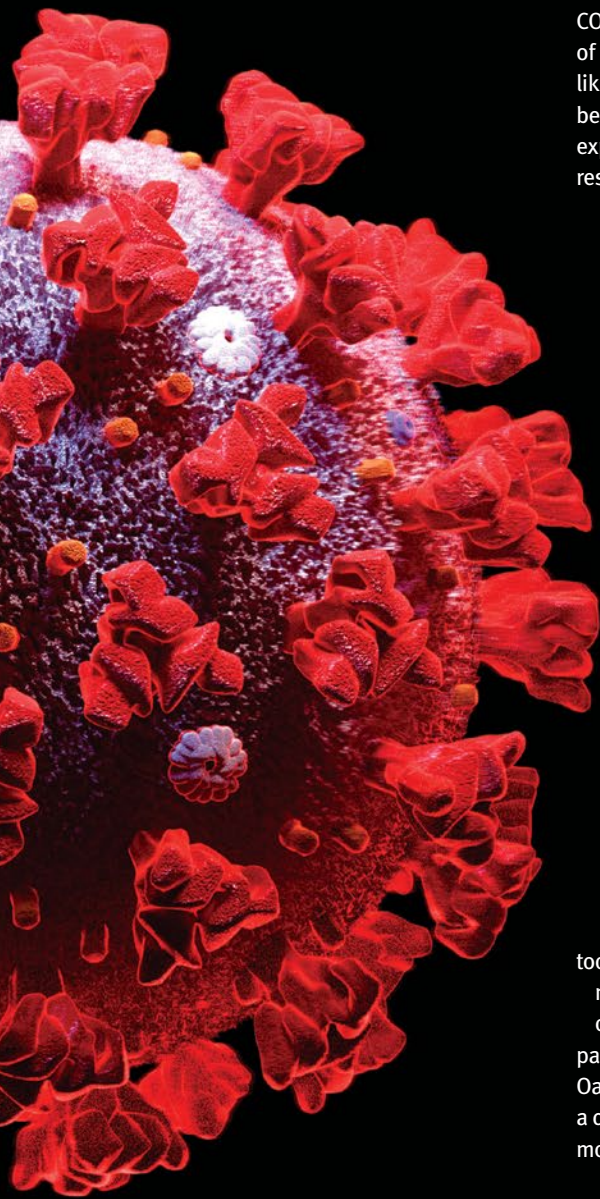
When the virus hit the United States in force, Los Alamos did what many other organizations across the nation did: sent most of its workforce home. Apart from key national security personnel who continued to work onsite, Laboratory employees worked on laptops from home with various forms of connectivity software to keep their programs going. Of course, this approach had its limitations; for example, most scientists no longer had access to their laboratories or experiments. But far from giving up and watching soap operas in their pajamas, they instead answered a new call to serve the nation. Within just a few weeks, the Lab's considerable supercomputer resources and expert personnel were allocated to national COVID-19 research efforts, and a rush of new internal research programs were variously proposed, approved, and underway.

SARS-CoV-2, the virus that causes the COVID-19 illness, is similar to other coronaviruses, such as those that cause SARS and MERS. Like them, it sprang upon the world suddenly, and relatively little

could be known at the outset. There are questions about its history—how it emerged, over time and geography—that need to be answered. There are questions about its nature, such as how quickly it spreads and mutates, how often it kills, and whether or not it can re-infect. There are questions about its genomics—what genes or proteins might be targeted for vaccines and other treatments. There are questions of molecular structure—what proteins the virus constructs itself from, what shapes they take, and how their functions might be inhibited by different molecules—molecules that could serve as effective drugs, as long as they don't introduce any toxicity themselves.

These sorts of questions require a tremendous amount of computational processing: examining one gene after another, checking every protein, screening vast numbers of existing and hypothetical drug molecules for both efficacy and safety. Whether by traditional large-scale data processing or advanced machine-learning techniques, high-performance computing enables rapid progress, perhaps condensing the timescale for the development of a vaccine or drug treatment. And supercomputer-based studies involving bioinformatics and molecular modeling have long been a specialty of Los Alamos National Laboratory. When the White House in mid-March announced a broad public-private coalition to support





supercomputer research in the fight against COVID-19, Los Alamos—joined by a number of other national laboratories, NASA, and the likes of Amazon, Google, and IBM—proudly began sharing its considerable hardware and expertise with the entire national COVID-19 research enterprise.

In addition, while the country was largely closing down, Los Alamos scientists were massively spooling up a whole host of important research initiatives. Some are focused on the virus itself: its origin, its natural history, and its rate of evolution. Some are focused on direct vaccine development—against SARS-CoV-2 specifically or coronaviruses broadly, potentially to protect against future emergent pathogens. Others seek to help with testing and treatment activity, including investigating ways to increase the supply of necessary medical equipment (e.g., ventilators and face shields), such as 3D printing new equipment or sterilizing existing equipment for reuse. Still others are focused on epidemiology: forecasting the virus's geographic and demographic spread and developing ready-to-use tools for informed, nearly real-time decision making in response to the evolving pattern of infection. Indeed, the Laboratory is partnering with Sandia, Argonne, and Oak Ridge national laboratories to produce a comprehensive, high-resolution pandemic model, integrating data collection and analysis

to support policy makers. Los Alamos is also working with partner infectious-disease laboratories in countries such as Jordan, Uganda, the Republic of Georgia, and others for monthly exchanges of information on COVID-19's genomics and molecular biology.

Several lines of research seek to analyze non-pharmaceutical mitigation strategies. How effective can we expect initial countermeasures, such as school closures and social distancing, to be over time? What about alternative strategies, such as more rigorous quarantines, with or without state-by-state variability? How will various scenarios affect rates of infection and death? Or the availability of key hospital resources, such as ventilators and healthy medical staff? And how can those resources be managed to optimal effect? Until drugs or vaccines are developed and distributed, answering these questions holds the greatest hope for minimizing the damage wreaked by SARS-CoV-2.

A global pandemic calls for two types of response. One is mass isolation, to protect individuals and slow transmission. The other is mass mobilization, to develop mitigation strategies, manage resources, and find a cure. When COVID-19 arrived, Los Alamos leapt into action on both fronts. **LDRD**

—Craig Tyler

In-depth coverage of Los Alamos research to combat the COVID-19 crisis will appear in the next issue of *1663*.

NUCLEAR NONPROLIFERATION

Centrifuge Sentries

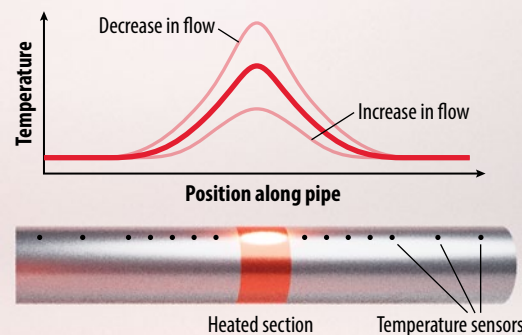
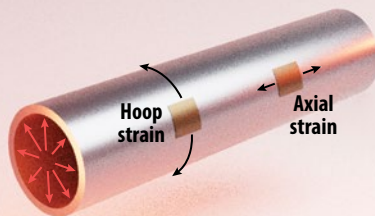
Inspectors need robust and reliable instrumentation to ensure that nuclear enrichment facilities are used for peaceful purposes.

What is happening inside the world's uranium enrichment facilities?

It is the job of the International Atomic Energy Agency (IAEA) to verify the peaceful use of special nuclear material. The IAEA deploys teams of inspectors, partially trained at Los Alamos, to gas centrifuge enrichment plants (GCEPs) to ensure that the plants are only producing low enriched uranium (LEU, suitable for nuclear power production but not weapons)—and in declared quantities—not highly enriched uranium (HEU). They use a suite of instrumentation, including an on-line enrichment monitor (OLEM), to verify the production of LEU for domestic nuclear power. These inspectors may be okay with a proliferation of acronyms, but not a proliferation of weapons-grade nuclear material.

A GCEP, working with uranium in the form of uranium hexafluoride gas (UF_6), separates the fissionable isotope uranium-235 from other isotopes in natural uranium, which contains less than 1 percent U-235. Standard enrichment results in a few percent U-235—that's LEU. But with certain illicit modifications, the enrichment can exceed the 20 percent threshold for HEU, and such undeclared enrichment could take place in a small corner of the GCEP. To determine the relative U-235 enrichment, an OLEM combines gamma-ray spectrometry with indirect gas density measurements. However, those density measurements rely on temperature and pressure measurements, the latter of which generally come from separate instrumentation controlled by the plant operators, not the OLEM itself. Furthermore, since almost everything happening inside of a GCEP is considered commercial proprietary or sensitive information, the IAEA and the plant operators have to agree on a monitoring regime that allows the IAEA to verify an operator's declaration while also protecting its sensitive technology.

Sensing gas pressure inside a pipe from the outside: With sufficiently sensitive sensors, the measured hoop and axial strain—expansion or contraction in the circumference and along the length of the pipe, respectively—reveal subtle changes in the pressure difference between the interior and exterior of the pipe. (Simultaneous measurements of strain along the circumference and length of the pipe capture the confounding effects of thermal expansion, allowing them to be subtracted out.)



Sensing mass flow inside a pipe from the outside: The effect of a localized heat source on pipe temperature up- and downstream depends on the rate of mass flow inside the pipe; more flow lowers the temperature on the outer surface of the pipe.

In real-world operation, both devices would be self-contained inside an insulating, tamper-proof casing.

“GCEP monitoring is a complex task, especially in less-cooperative environments,” says Rollin Lakis, a Los Alamos nuclear safeguards scientist. “To monitor a centrifuge plant with confidence—and what’s the point otherwise?—requires independent and trusted measurements of different process variables, including the pressure inside the UF_6 -carrying pipe. A new method to measure the mass-flow rate at many different locations in a GCEP would enable significant, near real-time design verification against facility misuse scenarios.”

Lakis teamed up with Los Alamos colleague Alessandro Cattaneo, a mechanical engineer with expertise in heat transport, modeling, and complex sensor systems. The devices Lakis and Cattaneo have in mind must be noninvasive, mounting onto an existing pipe rather than being built directly into the gas flow, if they are to be used at many locations within a GCEP. They have to be self-reliant, obtaining the pressure and mass flow inside the pipe using only the data they collect from the outside. They have to be connected to other devices around the plant and to IAEA inspectors’ information stream. And they have to be easy for inspectors to install and maintain.

So Cattaneo, Lakis, and other collaborators designed two different devices aiming at measuring the flow pressure and the flow rate from the exterior of a UF_6 -carrying pipe.

One collaboration, with Marcelo Jaime of the Materials Physics and Applications division at Los Alamos, resulted in a device that determines the internal pipe pressure (relative to the external atmospheric pressure) based upon strain measurements taken on

the outer surface of the pipe—i.e., the utterly minuscule amount by which the metal pipe itself expands or contracts in response to the pressure difference. To obtain a sensitive enough strain measurement, they integrated an ultra-sophisticated infrared laser-based fiber-Bragg-grating (FBG) interferometer, which detects stretching in the pipe metal at the level of tens of parts per billion, or equivalently the length of approximately ten iron atoms along the circumference of tested pipes.

“Our simulations and feasibility studies showed it was possible,” says Cattaneo. “So we built a mockup device to try it out. For pressures of interest in appropriately stiff aluminum and steel pipes, we have already obtained about 5 percent internal pressure-measurement sensitivity.” That’s good but not good enough. Lakis, Cattaneo, and Jaime are currently working to get the sensitivity down to 1 percent or better.

“A strategy to improve resolution by at least a factor of ten, possibly even 100, in the FBG interrogation has been identified in a new technology currently under consideration,” reassures Jaime.

The second collaboration, carried out with Robert Goldston of the Princeton Plasma Physics Laboratory, led to the creation of a noninvasive and operator-independent thermal mass-flow meter. The prototype applies a temperature gradient along the length of the outer surface of a gas-carrying pipe. The device correlates the internal mass-flow rate with external temperature and heat power measurements. In its simplest embodiment, with a single heater wrapped around the pipe, the more gas is flowing, the

greater the cooling effect on the pipe. “Our team showed that a 1 percent mass-flow-rate accuracy is within reach,” says Cattaneo.

“We have a little farther to go yet,” says Lakis, “but the good news is, we’ve already demonstrated that these methods work effectively. We have confidence that we can get the rest of the way there.”

We have confidence: and that’s exactly the point. **LDRD**

—Craig Tyler

SPACE

Space Changes Everything

Improving space travel by studying the gut microbiome and more

Microgravity may exert tiny forces, but its relative impact can be significant. Humans and other earth-bound organisms have evolved with the constant pull of Earth’s gravity. As such, long-term exposure to a lack of gravity—or a minuscule amount known as microgravity—leads to problems like muscle loss and decreased bone density in astronauts. Additional potential problems, such as how microgravity affects human digestion, remain underexplored. This is in part because the digestive system is complex and works in tandem with billions of microorganisms that live in the gut, which are collectively known as the gut microbiome. To further investigate the effects of microgravity on this complex environment, the Defense Threat Reduction Agency funded a collaborative project between Los Alamos biologists Armand Dichosa and Anand Kumar and scientists at Rhodium Scientific, LLC. The team launched its first human gut microbiome experiment in March 2020 on the SpaceX-20 mission from NASA’s Kennedy Space Center.

Over decades of space travel, experiments have shown that many types of bacteria behave differently in space than on Earth. Some harmful bacteria, for example, can become more pathogenic, while others grow

more slowly and are less pathogenic. This unpredictability has vexed the scientists tasked with keeping astronauts healthy. Some scientists theorize that the reason for this unusual behavior is because microgravity causes changes to the fluid environment in which the microbes live (e.g., saliva or stomach fluid). When the microbes don’t encounter “normal” fluid shear forces from their surroundings, they are not receiving the correct cues for their behavior.

Astronauts enter space with a diverse population of bacteria in their gut microbiomes. Because they are only allowed to eat specific sterile food and drink sterilized recycled water—both of which lack the normal assortment of bacteria—astronauts have limited exposure to new bacteria while in space. This makes it easy for their microbiomes to develop an imbalance and can result in various disease conditions. On Earth, the gut microbiome has been shown to impact many aspects of human health, so understanding how microgravity might alter the microbiome is critical to protecting people operating in space.

The Los Alamos samples that were launched in March contained bacteria isolated from fecal donors with healthy gut flora. These bacterial flight samples were carefully prepared so that each culture would have a complementary sample remaining on Earth. Once they arrived at the International Space Station, the cultures were grown under specific conditions and preserved. Upon their return to Los Alamos, both sets of samples will be sequenced and analyzed to help the scientists identify any changes in the bacterial communities’ genomic signatures.

“With this information, we may be able to prepare specific probiotics that could help astronauts

remain healthy while they’re in space,” explains Kumar.

The impact of microgravity on human health has clear implications for long-term space travel. But the peculiar behavior induced by microgravity that has been observed so far inspires scientists to study more—from other living organisms to inanimate chemicals and materials. With a view towards expanding this type of research, the Los Alamos Center for Space and Earth Science (CSES) recently allocated special funding for projects that could lead to further studies on flights from the Spaceport America launch facility in southern New Mexico. The new research topics range from detecting urinary-tract infections to studying plant growth to exploring space-based manufacturing.

All together, these projects help pave the way for a deeper understanding of microgravity. This knowledge will not only improve the health and well-being of humans on long-term space visits; it could also help scientists harness the power of microgravity for a wide range of new applications valuable here on Earth.

—Rebecca McDonald



NASA astronaut and Expedition 62 Flight Engineer Andrew Morgan retrieves gut microbe samples from a science freezer for the Rhodium Space Microbiome experiment to understand how microgravity enriches or depletes the microbes that affect astronaut health. CREDIT: ISS



The Advantage of Uncertainty

Physicist **Patrick Coles** develops algorithms to make quantum computing a practical reality and to unveil the boundaries of the quantum world.

IF YOU ZOOM IN ENOUGH—a single water molecule, say, instead of a pond—the world loses its familiar focus. Old certainties, like the location and motion of an object, become uncertain. Distinct physical attributes, like clockwise or counterclockwise rotations, become blurry mixtures, a little of each. The equations of physics no longer tell you what will happen, but rather the probabilities for everything that could happen. And even after one of those possibilities materializes, there's no way to explain why it happened, even with hindsight. Our usual notions of a deterministic reality are ambiguous at best, or at worst, downright meaningless. Up close, the “real” world gives way to the quantum world.

This quantum world is my world. It is where I live my professional life.

Don't get me wrong: I'm not asking for your sympathy. I like it here. I know it sounds frustrating living all the time without certainty, specificity, or predictability, especially if you're trying to get work done—and I do technical, computational work. But there's a silver lining here. As in other areas of life, with my work, there's something to be said for nuance, open-mindedness, and relaxing my need for control. Even for a task as detailed and precise as mathematical optimization or simulation, it can actually be a tremendous *advantage* to work without certainty, specificity, or predictability. In fact, a big part of my professional work, quantum computing, expressly relies on uncertainty. And I'm proud to say that my colleagues and I at Los Alamos have made incredible progress in this field in the past couple years.

Quantum software for quantum hardware

First things first: quantum computing is no longer just some future fantasy like starships and teleporters. Quantum computing exists. For very

simple computations, it actually works right now. And quantum computers—these are physical machines, currently available—are rapidly improving. Within a few years, these early-generation quantum computers will begin outperforming the world's most advanced nonquantum, or classical, computers when solving certain kinds of problems.

Now, as you may already know, a quantum computer bit, or qubit, is not necessarily a one or a zero; it can be some of each. In general, it is a shifting mixture, or superposition, of “oneness” and “zeroness.” Sometimes it's more one than zero, sometimes more zero than one, and sometimes fifty-fifty. If two qubits interact with one another, they can be in a superposition together, and that's what physicists call entanglement. This is like two light switches either both being on or both being off, but never one off and the other on. But it's more intricate than that, because you have the freedom to put a plus sign or minus sign in the superposition, which gives rise to interference effects (much the way colliding ocean waves or sound waves interfere, with peaks and troughs amplifying or canceling each other out).

Taken together, superposition and entanglement lead to an enormous number of possible states for qubits (and hence a quantum computer) to be in. By contrast, having a computer made of classical bits is like being confined to a prison. Imagine living in this incredibly huge space (the quantum world). To solve some important problem, like simulating the molecules in a coronavirus, you need to move from point A to point B in this huge space. So, with your quantum computer, which is completely free to move in this space, you simply take the straight-line trajectory from A to B. But with a classical computer, your movement is restricted; you are confined to the prison hallways, so you can't take the optimal path, and the calculation takes longer.

It is a common misconception that quantum computers simultaneously explore many different classical pathways at the same time. This is wrong. Ultimately, I believe that the quantum computer is the most difficult-to-explain technology ever invented, and I don't want to give a false explanation for why it performs certain calculations quickly. Rather, I like to turn the question around and ask: why are classical computers so bad at certain tasks? It's because using your laptop computer is like being confined to a prison, in the vast quantum world that we live in.

But it's not all about the hardware. Different kinds of algorithms are needed to take advantage of this very specialized hardware. For example, quantum computers offer a larger set of logical gates. Some of these mimic classical gates, such as AND, OR, or NOT, but others are exclusive to quantum computing and require new algorithms to use. You also need ways to optimize all the programs you try to run. For example, you don't want to waste limited quantum-computing resources on subroutines that are better handled by a classical computer chip, so you need specialized algorithms to parse that out. My colleagues and I have developed several algorithms of this sort.

Why are quantum-computing resources limited? Two reasons. The first is simply that the quantum computers that exist today have few qubits

to work with. State of the art right now is a 53-qubit machine from IBM and similar-sized machines from Google. The number of qubits available will certainly improve with time, but they remain limited now.

The second reason is more fundamental. Quantum superpositions are delicate. They can be ruined (or "collapsed" in quantum lingo) not only when they are deliberately probed (for example, by a scientific measurement) but also by any number of prosaic interactions with the environment, such as encountering a stray blip of electromagnetic radiation. Stray blips of this sort are ubiquitous (heat waves, radio waves), and particles in

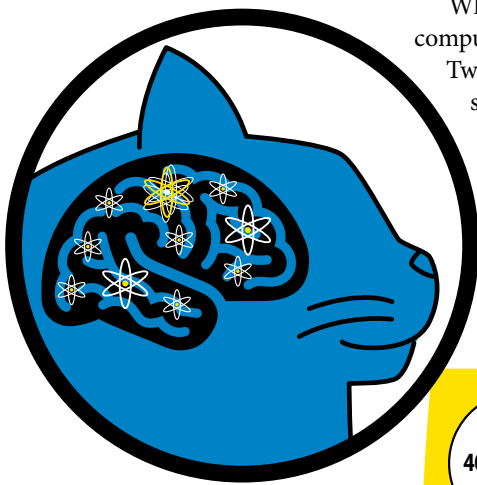
It can actually be a tremendous advantage to work without certainty, specificity, or predictability.

superposition states—such as a superposition of two different spin states, representing a superposition of 0 and 1 for computational purposes—can be shielded from the environment for only so long. Better methods for isolating qubits from the environment will presumably emerge over time, but nonetheless, the essence of a quantum computation is necessarily time-limited. A superposition can't be maintained forever, and if it collapses too early, the calculation is gone.

Quantum bits for quantum leaps

If qubit superpositions can be maintained long enough, however, they can be applied to certain classes of calculations that are severely impractical for a classical computer. A simple example is the purely mathematical operation of factoring—identifying the prime numbers that, when multiplied together, result in a given number (as $3 \times 2 \times 2$ is 12). Modern encryption methods, like those that make it safe to enter your credit-card information on a respectable website, rely on the computational difficulty of factoring. Breaking the encryption requires factoring numbers so large that it would take centuries or more for today's best classical computers to do. That's because a classical computer can't exploit the wavelike nature of the factoring problem (finding factors is like finding the periods of a wave) the way a quantum computer can.

Not surprisingly, another task at which classical computers dramatically underperform quantum computers is running simulations governed by quantum physics. Suppose for example you want to analyze a group of 53 electrons (the same number as the IBM machine's available qubits), and you're only interested in the very simplest property of each electron: its spin.



In a quantum superposition, multiple possibilities are simultaneously true. Unlike problems in classical physics, such as calculating the trajectory of a baseball, future outcomes in quantum physics are uncertain; they can only be assigned probabilities.



When measured with respect to a particular axis, electrons have only two spin states, called “spin up” and “spin down.” It’s binary—at least, in a collapsed, non-superposition state. That means the number of possible combinations is 2^{53} .

To track all that with a classical computer would require 2^{53} bits of memory, which is roughly a petabyte. Today’s most advanced supercomputers can handle that, although even high-end consumer computers cannot. But add one more electron to the simulation—54 electrons instead of 53—and the memory requirements *double* to 2^{54} . Adding just a few more electrons takes us beyond the capability of the most powerful classical computers currently in existence—all to simulate the most simplistic binary spin states of just fifty-some particles! I mean, imagine working with the more complicated states of electrons within atoms, which have various energy levels and orbital properties in addition to spin. Then 2^{53} could become something more like 20^{53} . Besides, 53 particles might represent a single molecule, and not a very big one; by contrast, a bit of matter you could hold in your hand and notice would be upwards of a trillion trillion particles.

The essential trouble here is that these types of problems scale exponentially. Add just one more digit to the number being factored or one more particle to the quantum simulation, and the amount of memory required doubles (at least). Just a 2 percent increase in complexity (from 53 to 54 electrons, say) results in a 100 percent increase in computational difficulty and memory requirements. (By now, everyone is familiar with the accelerating pace of exponential growth after seeing the horrific, rapid rise of the coronavirus pandemic.)

The same is not true with qubits. Each qubit can simulate one electron’s spin. Going from 53 to 54 electrons doesn’t double the number of qubits required; it just means adding one more qubit. And that’s the key advantage of quantum computing. It eliminates the exponential growth in computational difficulty that classical computers face with these kinds of problems. Instead, the growth is linear, so that a marginal increase in a problem’s complexity produces a correspondingly marginal increase in computational difficulty. That’s what makes quantum computing so promising. It’s also what makes the whole field so fascinating: the way to obtain mathematical certainty in the face of intractably expanding complexity is to deliberately introduce additional uncertainty with superpositions of qubits.

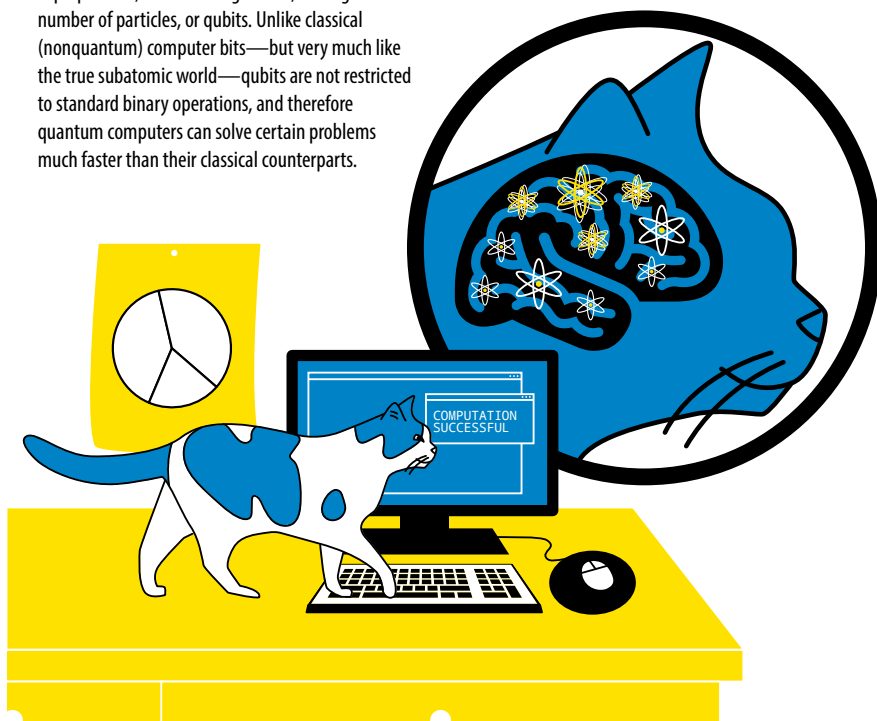
Quantum simulations for quantum behavior

I used to find it bizarre that physics has two distinct and seemingly incompatible ways of describing nature. When studying just one particle or a few, quantum physics is necessary and reliable. When studying larger systems of particles—bacteria, airplanes, galaxies, whatever—classical physics is obviously the way to go, and quantum physics, while perhaps still true if you could somehow account for all the constituent particles, is wildly beyond our ability to calculate and utterly unnecessary.

While superimposing human perspectives onto nature invites boundaries like this, physicists like me much prefer smooth transitions rather than abrupt changes.

Now, like most physicists, I believe that the boundary between quantum and classical lies in a process called decoherence. A quantum system “decoheres” by broadcasting information about itself to its environment, and then classical physics

Quantum computing relies on maintaining a shared superposition, called entanglement, among a small number of particles, or qubits. Unlike classical (nonquantum) computer bits—but very much like the true subatomic world—qubits are not restricted to standard binary operations, and therefore quantum computers can solve certain problems much faster than their classical counterparts.



emerges. But how does that work? How exactly do the essential qualities of quantum behavior—superposition, entanglement, and uncertainty—conspire to produce rigid, predictable classical laws like Newton’s laws of motion or Maxwell’s laws of electromagnetism? Everyone in physics knows that understanding

For some calculations, the fastest way to obtain mathematical certainty is to deliberately introduce the uncertainty of qubits.

decoherence, and therefore the quantum-to-classical transition, represents a major scientific discovery, but there’s never been any rigorous way to test it.

That’s about to change. Current estimates suggest that decoherence really gets underway for systems of a few hundred particles. That’s enormously beyond the capability of any foreseeable classical supercomputer, possibly forever, due to the exponential-scaling problem. But a few-hundred-qubit quantum

computer is probably only a couple years away. So I've been working frantically to develop algorithms by which a quantum computer can simulate quantum decoherence. That way, we'll be ready when we, as a species, finally get the chance for the first time in history.

Amazingly, molecules around the few-hundred particle threshold for the quantum-to-classical transition show up often in the biochemistry of the human body. Most people think

Our algorithm identifies the onset of decoherence by constructing as-classical-as-possible descriptions of a quantum system.

that these molecules are so closely surrounded by others that they're effectively much larger sets of particles and therefore, in effect, permanently decohered. But we can't be sure. Many, many biomolecules are about the right size, such that quantum decoherence could possibly be integral to the processes they carry out—processes like sight and smell, neurotransmitter signaling, and DNA replication. We scientists may have sophisticated ways of modeling stellar interiors, rocket engines, and global climate dynamics, but we're only just now approaching the point of having the computational technology to understand ourselves.

Here's a case in point from a paper that several Los Alamos colleagues and I published last year. Proteins, including the enzymes that catalyze all sorts of biofunctions in all sorts of lifeforms, are generally larger than just a few hundred particles, but they're still expected to exhibit some remnants of quantum behavior. They are made from long chains of amino-acid molecules, but rather than remaining linear chains, they bunch up with a complex set of specific folds. How they fold is extremely important; the resulting shape is intimately connected to the proper function of the molecule.

So how do the proteins know how to fold properly? There's some debate about that. One theory argues for classical determinism: the chain of amino acids will kink and fold at the same spots every time because of some complex set of built-in classical forces. But another theory argues that the proteins are solving an optimization problem from scratch, effectively running a quantum computation. They are exploring different ways to fold—at different locations along the chain, in different sequences—via some kind of composite superposition to arrive at an optimal endpoint.

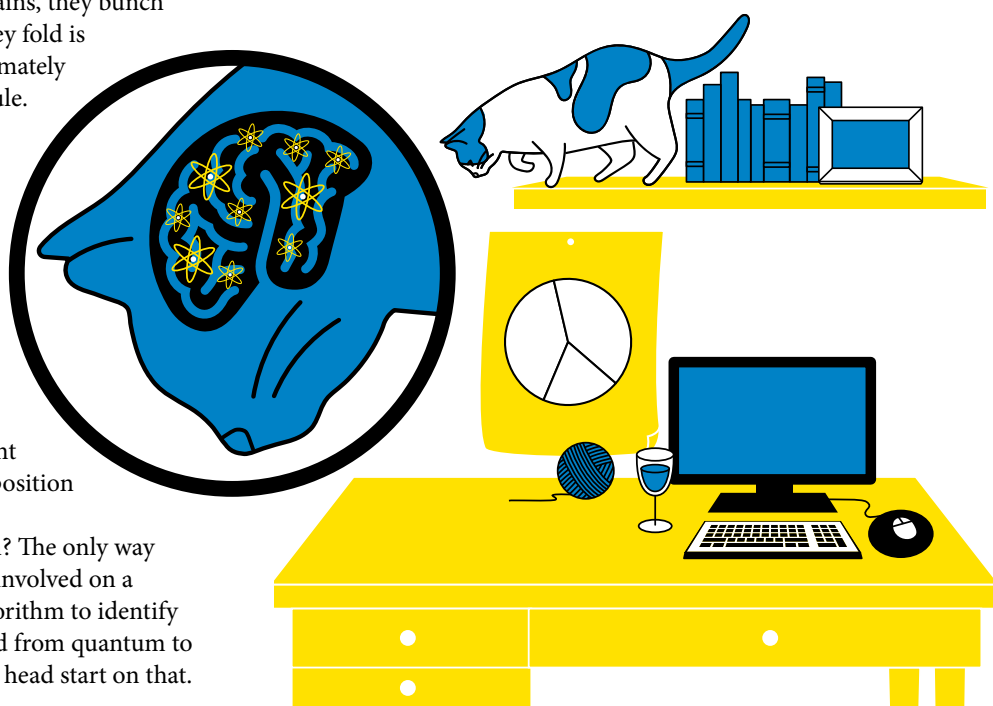
Wild conjecture? Or reasonable speculation? The only way to know for sure is to simulate all the particles involved on a quantum computer and apply a specialized algorithm to identify whether or not the relevant behavior has shifted from quantum to classical. As it turns out, we have a tremendous head start on that.

Quantum histories for the quantum-classical transition

I count myself fortunate to have worked under the tutelage of Professor Robert Griffiths during my first postdoctoral position ten years ago. Griffiths developed a powerful methodology for doing quantum physics known as the consistent histories (CH) formalism, and I learned a lot about this novel approach from him. It's not often used, partly because it is conceptually quite different from the standard quantum mechanics methodology taught to physics students, and partly because it quickly bumps up against the exponential-scaling problem when implemented on a classical computer. However, here at Los Alamos, I realized that CH offered a particularly promising way to study the quantum-to-classical transition on a quantum computer. My colleagues and I recently developed a hybrid algorithm—part quantum computing, part classical computing—to do just that.

The details are complicated, but in essence it works like this: First, you invent what's called a framework in the CH formalism. This is a series of observables, such as the individual atomic positions in a folding protein, measured individually in some order. This much, but no more, can be done on a classical computer. Then you use a quantum computer to check all the possible sequences of measurement outcomes, or "histories," for "consistency"—looking for sequences that can occur without interfering with one another. (In quantum mechanics, particles have wavelike attributes and can therefore interfere; we need to suppress this interference if we want to have a consistent framework.) The algorithm repeats this entire process to evaluate many different frameworks.

Quantum decoherence occurs when a large number of particles get involved, somehow "diluting" the superposition. A quantum computation can be maintained only as long as the entangled qubits are isolated from their surroundings, and when that is no longer true, the superposition is replaced with a single outcome. At this point, physical behavior appears classical, not quantum.



Now—and this is important—I’m from Pittsburgh. So I like to think of using consistent histories in terms of answering questions like, “What are the odds that both the Steelers and the Penguins win their respective championships this year?” The consistency here comes from the fact that the two events do not interfere with one another; both teams can (and absolutely should) win in the same year. Or one or the other. Or (gasp!) neither. CH seeks out frameworks like that—those with sets of outcomes not riddled with quantum interference. Effectively, this consistency search obtains as-classical-as-possible descriptions of a quantum system, which means it can assign scores rating “how classical” some process is. By finding the most consistent, most classical behavior, the algorithm can identify when and where decoherence is occurring.

Wow, right?

This algorithm is delightful in its apparent contradictions. It represents a sort of metaphorical superposition of nonoverlapping states: relying on both quantum and classical computations, maintaining a superposition of qubits to simulate the collapse of a superposition of particles, and calling upon purely theoretical foundations (consistent histories) to advance practical applications

conversely, to take advantage of qubit-based processing to compile quantum-computing algorithms—that is, translate them from a logical programming language used by programmers like me into machine-language instructions. We’re exploring the fertile intersection between quantum computing and machine learning. We’re proposing new algorithms to solve linear systems of equations (a ubiquitous task in engineering) on quantum computers with an exponential speedup. We’re improving quantum encryption technology and deploying new ways to assess its performance. And, of course, we’re attacking the problem of decoherence, hard. To me, all of this feels like a new kind of progress for humankind. We’re finally using nature’s fundamental methods, processing information the way nature does, and simultaneously exploring all possibilities in any situation.

Reality isn’t, well, real. Not in the way we normally think of it, anyway. Our reality emerges from something else, something expressly nonspecific. We’ve known this for a long time, but we’re only just now beginning to truly understand it, use it, and learn from it. We’re learning to accept ambiguity to obtain precision. We’re making unpredictability work to our advantage. We’re zeroing in on classical certainty by widening our view of quantum

We’re finally processing information the way nature does, no longer constrained by classical bits.

(quantum computing). Here in the quantum world (where I live, remember?), it’s like installing a window that looks out onto the so-called real world beyond—a window that lets us see not just *what* the classical world looks like, but *why* it came to look that way.

Superposition of progress

I’m relatively new to the quantum computing team at Los Alamos, having just started my fourth year. But I can’t believe how much we have accomplished together in that time. I should note that of course we’re standing on the shoulders of giants, and one particular giant deserves special mention: our colleague Wojciech Zurek, just down the hall, has been instrumental in pioneering a great deal of quantum foundations research, especially in the area of decoherence. Other Los Alamos colleagues include Rolando Somma, who is also developing functional quantum-computing algorithms for existing and future quantum computers; Andrew Sornborger, who is doing fascinating work in quantum and neuromorphic computing and is collaborating with me on the intersection between these two topics (so-called “quantum machine learning”); and Lukasz Cincio, Carleton Coffrin, and Stephan Eidenbenz, who have all worked with me in co-organizing a prestigious quantum-computing summer school that sees students from around the world come here to Los Alamos each year for training in the theory, application, and programming of quantum computers. (And those are just a few of my fellow staff members in this amazing group; I haven’t even mentioned the many talented postdoctoral researchers we have here!)

We’ve developed new codes to conserve qubit resources and improve quantum simulations and, perhaps somewhat

histories, and we’re solving difficult problems faster by expanding beyond the paths offered by classical bits. It’s a thought paradigm almost deliberately built on contradiction. And it’s completely new, except it’s not. We’re actively managing qubits and developing new ways to query them, but we’re also just obeying the standard wisdom of the ages. Embrace uncertainty. Live in the now. Hold on loosely, but don’t let go.

If you zoom out enough, the world loses its familiar focus. The same thing happens if you zoom in. **LDRD**

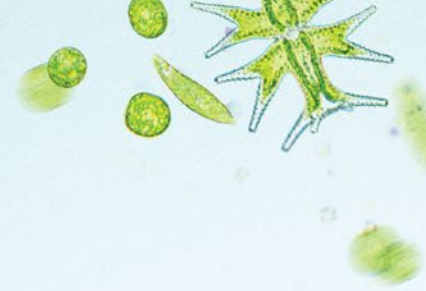
—Patrick Coles

MORE QUANTUM COMPUTING AT LOS ALAMOS

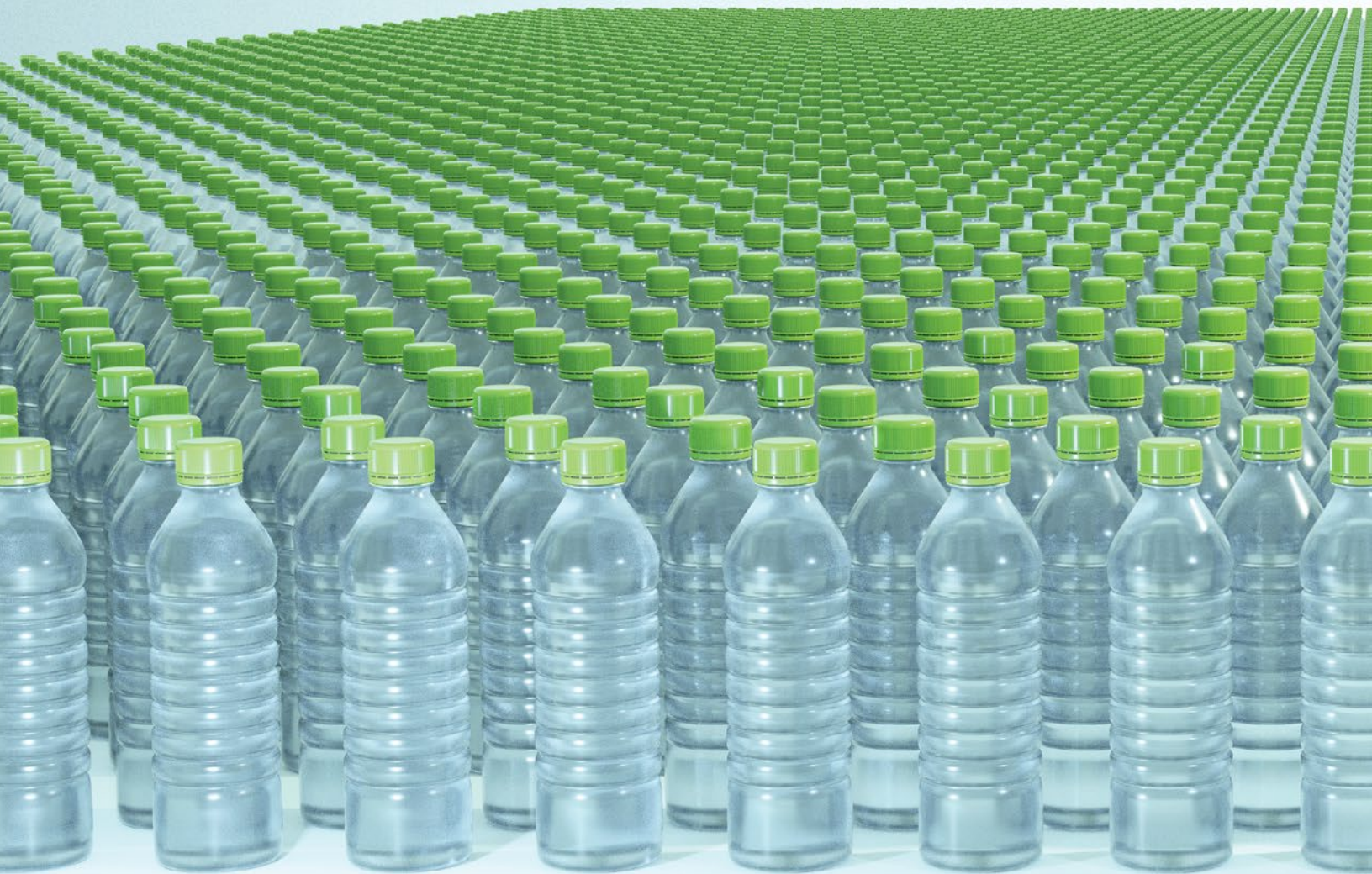
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MADE BY



A collection of various green, rod-shaped and spherical microorganisms, some with flagella, floating in the upper half of the image against a light blue background.

MICROBES

New plastics—produced by microorganisms and designed to degrade—stand to reduce the plastics pollution problem, one bottle at a time.



PLASTICS ARE PERFECTLY DESIGNED for every imaginable need. Some are strong and steadfast, others flexible and elastic. Plastics by definition can be molded into any possible shape and seem to be available for any plausible purpose. They are inexpensive to make and lightweight to transport. In fact, after millennia of human ingenuity, plastics are perhaps the ideal material. Except they're not.

Plastics are cheap to produce because they are byproducts from the production of fossil fuel-based gasoline, and there are associated costs. Fossil-fuel resources are limited, the production of plastics creates greenhouse gases that contribute to climate change, and when plastic products are thrown away—as millions are every single day—they litter landfills and oceans, where they will persist for hundreds of years.

Humans are faced with the stark reality that these materials, which seemed to magically transform modern life, are in fact a danger to the planet and its inhabitants. Plastic particles from deteriorating garbage are contaminating drinking water, showing up in the stomachs of sea creatures,

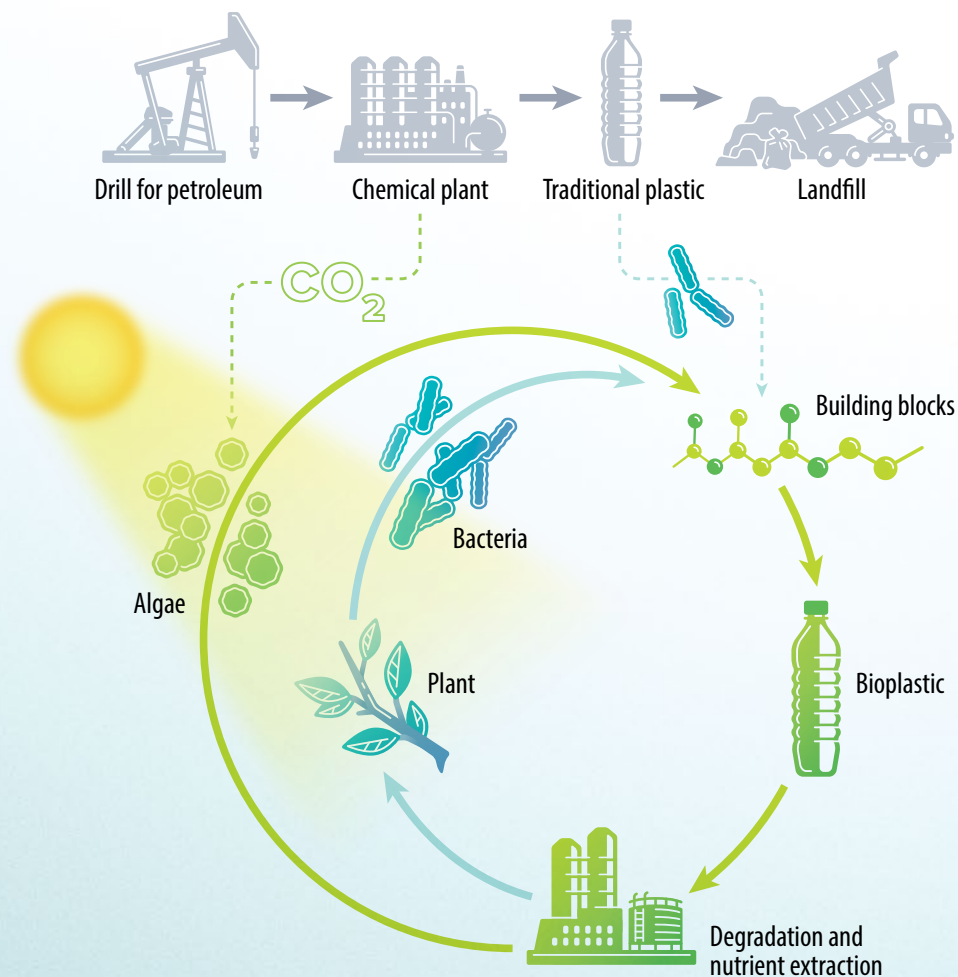
and making it up the food chain and onto our dinner plates. And, although awareness is rising along with the prevalence of re-usable water bottles, straws, grocery bags, and lunch containers, the plastics production lines have not slowed. Why? Because plastics are optimized for each product and purpose, and society is struggling to find suitable alternatives.

New strategies are needed to address this challenge. Humans cannot realistically remove plastics from their lives, but meaningful action is possible nonetheless. As many scientific solutions have been found by turning to nature for help, biologists at Los Alamos are working to build better plastics by engaging living sources of carbon, such as plants, and workhorse microorganisms, such as bacteria and algae. Their strategy combines experimental biology, chemistry, bioengineering, genomics, and machine learning to optimize every aspect of the plastic-production process. The goal is simple: the plastics of the future will be bio-based, biodegradable, and of course, perfectly designed for every imaginable need.

Making carbon cycle

Every minute of every day, one million plastic bottles are purchased. Water bottles, soda bottles, shampoo bottles, dish soap bottles... one million, every minute. These bottles are composed mostly of carbon, hydrogen, and oxygen atoms arranged as a long chain of identical sub-units called monomers, together forming a polymer. The monomer building blocks come mainly from fossil fuels, which in turn come from plants and animals that were decomposed and fossilized millions of years ago.

Plastics made from petroleum in a traditional "linear" economy (top row) are mostly sent to landfills and are slow to degrade in the environment. In a more circular "bioeconomy," products do not become waste but rather feed back into the system to become something else, or the same thing again. Plastic products would be produced by microorganisms using renewable sources: photosynthetic algae or bacteria that metabolize plants. The new plastics would more easily degrade if discarded but could also re-enter the economy through deliberate industrial degradation and nutrient extraction. The dotted lines show the potential for further sustainability—by capturing greenhouse gases, such as CO₂ or methane, from industrial processes to feed to algae and by using bacteria to degrade traditional plastic materials into useful building blocks for manufacturing.





Discarded plastics in landfills and oceans break down into smaller and smaller pieces, known as microplastics. Microplastics are generally less than 5 millimeters in length and have been found contaminating drinking water, in the stomachs of sea creatures, and making it up the food chain onto our dinner plates. In fact, some studies suggest that the average person now consumes 5 grams of plastic—roughly the equivalent of ingesting a credit card—each week.

The strong carbon bonds that are created during the polymerization process make plastic difficult to break apart, which is one reason it is so useful. As a result, discarded plastics in landfills and oceans just break down into smaller and smaller pieces of plastic, known as microplastics, and don't easily decompose back into their monomer building blocks to be usefully incorporated into either the ecosystem or the economy.

Plastics can be recycled once or twice, but overall very few plastic products are recycled at all—less than 10 percent by some estimates. Furthermore, most are *downcycled* into items of lesser economic value such as furniture stuffing or carpet. If plastics could be *upcycled* into higher-value items, such as sports equipment or auto parts, there would be incentive to invest in recycling infrastructure and to manufacture items with recycled material.

they feed back into the system to become something else, or even the same product again. A bioeconomy is this same concept but driven by materials that are derived from biological sources or made through biological processes. These economic ideas mimic nature's carbon cycle: Most carbon-based materials such as wood and cotton are naturally recycled in the environment when microorganisms decompose them and move carbon molecules from one form to another. When it comes to plastic, however, the carbon cycle is stuck: plastic just stays plastic for too long.

But not all plastic needs to last forever. While some plastics, like the dashboard of a car, must continue to be strong for decades, single-use plastics don't need to be as robust. The challenge is to figure out the components of a bioeconomy for plastics: What plastic-like materials can be competitively made for various

WHEN IT COMES TO PLASTIC, THE CARBON CYCLE IS STUCK

Alternatively, corn and sugar cane can be used to generate “bioplastic” polymers, such as polylactic acid (PLA), that can be made into cups, cutlery, and containers. These and other bioplastics don't use fossil fuels; however, their production competes with food resources and the polymers are still difficult to break down. Traditional recycling facilities cannot process most bioplastics, so they must be taken to industrial composting facilities, which are not widely available.

“Just because something is made biologically does not mean it is going to degrade faster,” says Babetta Marrone, Los Alamos biologist. “There may be some greenhouse-gas advantage, but they're not contributing to a more circular economy that could free up the carbon for other applications.”

The idea of a circular economy is to make products that do not become waste, but rather, after their intended use is complete,

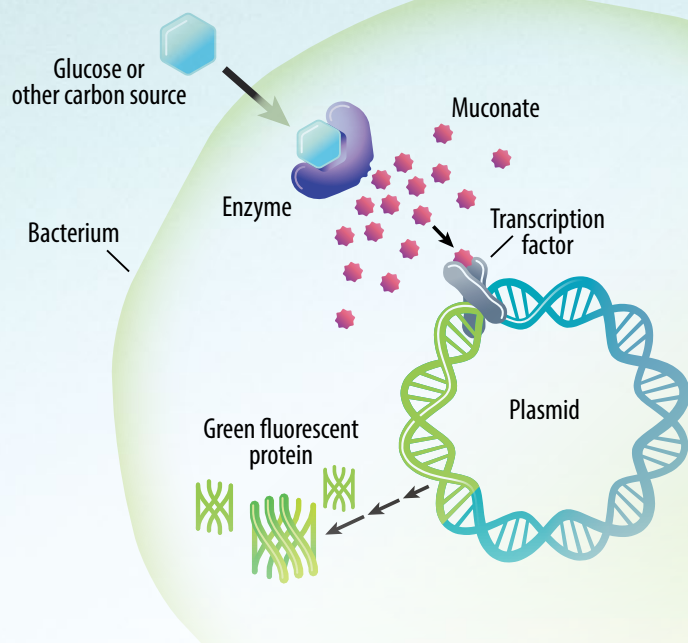
purposes and also degrade when appropriate? Microorganisms are key to nature's cycle of breaking down and reconstructing carbon—and as such they will be key to a future bioeconomy as well.

Glowing green

In the 1920s, French microbiologist Maurice Lemoigne studied the organism *Bacillus megaterium*, which naturally produces a plastic-like polymer and uses it to store energy. *Pseudomonas putida* is a bacterium discovered in the 1980s that can metabolize benzene, toluene, and other aromatic hydrocarbons that are hazardous to the environment. In 2016, Japanese researchers isolated another bacterium that can break down and metabolize plastic; they found it outside a bottle-recycling facility.

Envisioning that microorganisms could be harnessed to degrade plastic waste is one thing, but optimizing them for a

Computational biology is used to evaluate the structure of proteins called transcription factors in order to create a new transcription factor that matches and perfectly binds to muconate, a useful building block of nylon. The transcription factor is added to a specific point on a circle of DNA called a plasmid, at the beginning of the gene for green fluorescent protein (GFP). The plasmid and transcription factor are added to *P. putida* bacterial cells, and when muconate is produced and begins to accumulate, some of the muconate molecules bind to the transcription factor, causing it to signal enzymes to transcribe the GFP gene. Once the gene is transcribed, the cell begins to synthesize GFP molecules, and as more muconate is made, more GFP accumulates. Scientists can rapidly screen the cells using a laser that makes the GFP glow green; the cells that have the most GFP will glow the brightest, allowing the scientists to identify and separate the cells that make the most muconate.



large-scale clean-up—picture the 1.6 million-square-mile plastic patch in the Pacific Ocean—is a challenge. Furthermore, scientists have studied multiple microorganisms that naturally produce carbon-building blocks similar to those found in transportation fuels and plastics. However, to compete with fossil fuel-based production, these organisms would need to thrive under industrial conditions.

“The natural enzymes that break down plastic waste are not efficient and need to perform faster,” explains Taraka Dale, biologist and Biomass and Biodiversity team leader at Los Alamos. Through bioengineering, scientists can improve enzymatic activity—such as enabling enzymes to perform at

bacteria that have been identified as good strains for biomanufacturing. The consortium adopted *P. putida* because of its tolerance for extreme conditions and its ability to digest aromatic hydrocarbons such as toluene into a useful molecule called muconate, which the bacterium naturally produces during metabolism.

Muconate can be converted to adipic acid, which is a building block of nylon. BioFoundry partners at the National Renewable Energy Laboratory (NREL) began engineering *P. putida* to improve its ability to use glucose from plants, instead of toluene, as food to make the bacterium produce the building blocks for bio-derived nylon. Next, the Los Alamos team contributed

THE PLASTICS OF THE FUTURE WILL BE BIO-BASED AND BIODEGRADABLE

the high temperatures needed for industry—and fine-tune cellular production of various building blocks for new plastics. However, in order to succeed, they need sensitive and accurate ways to “see inside the cells” to determine which enzymes are working properly.

Dale and a number of Los Alamos colleagues are partners in two Department of Energy-funded consortia—the Agile BioFoundry and BOTTLE (Bio-Optimized Technologies for keeping Thermoplastics out of Landfills and the Environment)—focused on developing bio-based manufacturing and deconstructing plastic waste. For both consortia, one of the main contributions from the Los Alamos team is a revolutionary biosensor, called Smart Microbial Cell Technology, that allows the scientists to screen bacteria and select the varieties that perform best.

As part of the Agile BioFoundry, the Los Alamos team develops these performance-screening tools for new strains of

its biosensor as a reliable, sensitive way to figure out which candidate cells were performing best. The biosensor is added to all candidate cells and causes the ones that produce the most muconate to “self-report” by glowing green (see graphic above).

“Using the biosensor, we can screen thousands of variables in one tube at one time,” says Dale. “And in this application, all of them are reporting production of the target molecule, muconate.” In their most recent studies with NREL and Oak Ridge National Laboratory, the team reported three-fold improvements over other systems to create bio-derived muconate.

Furthermore, because the biosensor can be tailored to report many types of activity within a cell, it is being used for many different projects. As part of BOTTLE, the biosensor will be used to develop microbes that deconstruct traditional plastic into its building blocks, which can then be upcycled into higher-value products.

The elephant in the room

One of the first plastics ever developed was invented in 1868 as a way to save the elephants. At the time, the game of billiards was gaining popularity and people feared the ecological impact of making more and more billiard balls out of ivory. Hoping to win a \$10,000 award for finding an ivory substitute, an inventor named John Wesley Hyatt made billiard balls out of something completely different: cellulose nitrate, or celluloid. In an attempt to save one precious natural resource, an entirely new class of materials was invented.

Something disruptive is needed again. Using microbes to make plastics or degrade plastics is one solution to the plastics problem; however, many agree that a better solution would be to develop completely novel kinds of bioplastics that are intentionally designed to degrade at the end of their lives. Furthermore, new types of plastic molecules may even have advantages over fossil fuel-derived ones.

In 2018, Marrone convened a multi-disciplinary team of scientists at Los Alamos to explore this challenge in a project called BioManIAC (BioManufacturing with Intelligent Adaptive Control). Inspired by MANIAC, the pioneering first computer at Los Alamos, Marrone and her team are using biology, chemistry, and machine learning to create a process for finding entirely new plastics. Their goal is to identify monomer building blocks that are made using photosynthetic microbes such as algae and that readily return to the ecosystem as the plastic degrades, eliminating the need to collect and recycle waste materials.

Why the switch to algae? As Dale puts it: “Instead of growing plant biomass in order to feed and grow bacteria, it is more sustainable to use photosynthetic microbes directly.” Algae can grow outdoors using minimal infrastructure and non-potable or saline water, and they can even use waste carbon dioxide (CO₂) from a nearby industrial plant, rather than simply venting the greenhouse gas into the atmosphere. As long as they have these ingredients—sunlight, water, and CO₂—the algae use photosynthesis to produce carbon building blocks.

Bio-derived molecules have diverse functionalities, so many new kinds of polymers are possible. The challenge lies in deciding what makes a good bioplastic, then matching physical characteristics with their chemical makeup, and then matching those chemicals with the appropriate biological pathways.

“We can use machine learning to accelerate the process of biopolymer discovery, design, and development,” says Marrone. “We want to be able to say ‘I want to design out brittleness and design in elasticity, but at the same time make the product degrade faster.’”

Built to last... but not forever

The BioManIAC team is composed of experts in three scientific disciplines: chemistry, biology, and machine learning. Working together, the team members have begun to evaluate a few specific building-block molecules and the corresponding pathways for producing novel bioplastics.

To test their approach, the team is using cyanobacteria, which are simple, well-studied organisms that, like algae, use photosynthesis to make carbon-based molecules for energy storage. Some of these storage

molecules, called polyhydroxyalkanoates (PHAs), are already considered desirable for bioplastic production because they are biodegradable and can be used to make polymers with a wide range of plastic-like characteristics. However, much is still unknown about what combination of different PHA monomers is required for which specific plastic traits. The goal of the chemistry team is to evaluate these possibilities.

“Our team will systematically create and observe each monomer combination for physical and mechanical properties,” says Los Alamos polymer chemist Carl Iverson.

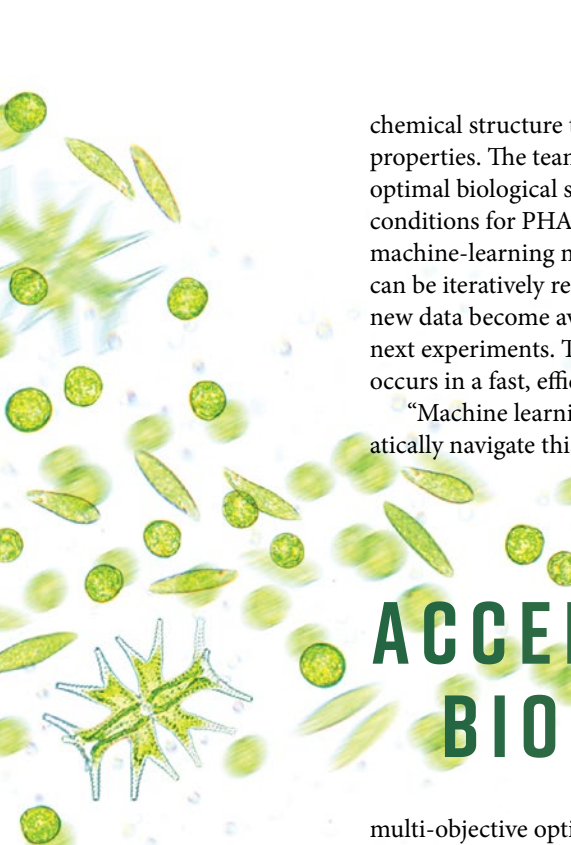
Specifically, Iverson’s team is screening PHA monomers for their thermal properties, such as melting point and glass transition temperature, which is the point at which a material transitions between a glassy and brittle state to a rubbery, flexible one. The team is also examining mechanical properties by doing puncture and elongation tests and measuring resistance to tearing. In these first BioManIAC experiments, Iverson is looking for polymers that can replace polyethylene and polypropylene, both of which are used for single-use plastics like grocery bags and cutlery.

To accelerate identification of the best candidates, Los Alamos machine-learning expert Ghanshyam Pilia and his team are combining Iverson’s experimental data with previously published data to develop, train, and validate a predictive machine-learning model that connects polymer



A cellulose nitrate, or celluloid, billiard ball invented in 1868 by John Wesley Hyatt as a potential replacement for ivory-made billiard balls. The ball pictured was gifted to the National Museum of American History by the Celanese Plastic Company.

CREDIT: Division of Medicine and Science, National Museum of American History, Smithsonian Institution



chemical structure to specific physical properties. The team also plans to identify optimal biological synthesis and culture conditions for PHA production. The machine-learning model is adaptable and can be iteratively refined and improved as new data become available, guiding the next experiments. This way, optimization occurs in a fast, efficient manner.

“Machine learning helps us systematically navigate this multi-parameter,

new plastics that could degrade into monomers fairly quickly in a landfill environment, allowing the building blocks to feed back into the natural carbon cycle. Alternatively, if collected, these plastics could be composted in an industrial environment and the building-block nutrients could be extracted and fed to algae, bacteria, or plants to be incorporated into new plastic products.

Although Iverson’s team is making test monomers in a chemistry lab, he explains that the chemical process isn’t scalable to industrial-level production—it’s too expensive and toxic. This is why a biological system for production is needed. Furthermore, the atoms in PHA molecules have a specific spatial arrangement

MACHINE LEARNING ACCELERATES THE PROCESS OF BIOPOLYMER DEVELOPMENT

multi-objective optimization problem,” explains Pilania. “We have a wish list of properties for biopolymers such as strength, flexibility, and biodegradability, but more often than not, these properties have trade-offs and sometimes strongly conflicting relationships. You can’t have them all optimized at once. The goal is to find the best-case scenarios hidden in this polymer-chemical space.”

Using additional experiments, the team is examining what environmental conditions are necessary to biodegrade the candidate polymers, what the polymers will degrade into, and whether or not those molecules will have a negative environmental impact. The goal is to have

(i.e., the angle at which the methyl group sits) that is very difficult to achieve in a chemistry lab.

“The biological process to make PHAs is exquisite,” says Iverson.

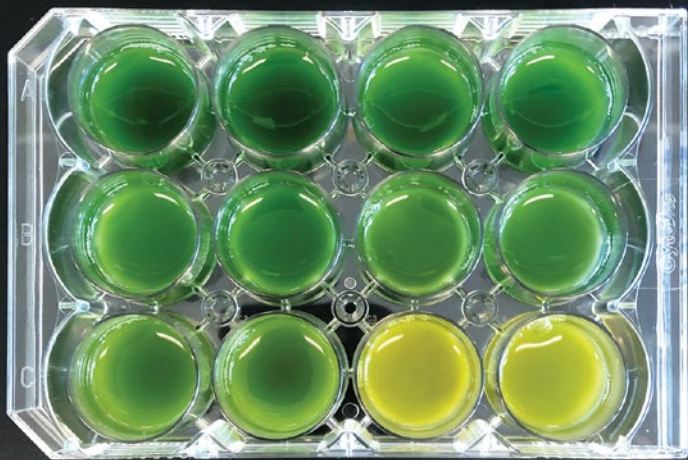
Instructions for production

Biology might be responsible for exquisite PHA production, but the process is hidden inside microscopic cells. In order to prepare cyanobacteria—and eventually algae—for industrial-scale production, scientists require a solid understanding of which genes and proteins are responsible for making PHA. Furthermore, if the chemistry team identifies specific PHA-like monomers that should be modified to make, for instance, a better plastic bag, then the biology team needs to decide if it’s biologically feasible to do so and how.

For decades, scientists have been able to sequence the genomes of living organisms to study the DNA blueprint that enables them to exist. The DNA broadly contains “coding”

Los Alamos biologist Sangeeta Negi checks on an algae culture, while the rest of the culture flasks shake on an oscillating table. For many years, Los Alamos scientists have been optimizing algae growth for biofuels and bioproduct development. This expertise is now key to developing the next generation of bioplastics.





Cyanobacteria cultured with different nutrients in different amounts result in distinct color changes. Using machine-learning-identified genes, the BioManIAC team will use these bacteria to test production of various building-block molecules for plastic biomanufacturing.

CREDIT: Ramesh Jha/LANL

and “non-coding” regions. The former is made up of genes—sequences of nucleotides that provide instructions for assembling amino acids, which align and fold in unique ways to form proteins that carry out specific functions in cells. The latter is the DNA found between genes, which used to be considered junk but is now known to contain valuable information about gene regulation.

Coupling genes with their functions is a laborious experimental process, so often the first step in understanding a new genome is to search databases for sequences that match known genes. BioManIAC scientists can search the databases to find genes that are known to make PHA; however, if they want to discover new pathways, or even new monomer products, they must explore the unknown territory in both coding and non-coding regions. To do so in the most efficient manner and without spending excessive time in the lab, the team is employing machine learning.

The BioManIAC approach is to start by looking for small pieces instead of entire genes or proteins: Instead of looking for a whole fish, they are looking for anything that resembles a fin. With this approach in mind, the team divides an organism’s genomic data into equivalent-sized pieces called “*k*-mers”: sections of DNA that are *k* nucleotides long. For instance, if *k*=14, then the algorithm would determine all possible 14-nucleotide pieces in an entire genome of interest (including non-coding areas) and compare those segments to all known genes associated with PHA production. Any *k*-mer match would indicate possible new PHA-related information that should be further investigated.

The team is also looking through the genomic data for code that matches that of specific PHA-related “protein families.” Protein families are small groups of amino acids that work together for a specific function, such as in the active site of an enzyme. Again, by searching for protein families instead of whole proteins, the scientists are looking for a match of only a small, but critical, piece of data. In essence if it looks like a fin, then there is the possibility it might be from a fish, and perhaps the right

kind of fish. If these protein families are found, they could lead to the discovery of new enzymes associated with PHA.

“We might first ask: Is the *k*-mer present in the data?” says Los Alamos biologist and Bioinformatics and Genomics team leader Shawn Starkenburg, “But then we go deeper: If the *k*-mer is present, does the organism also produce PHA? And next, is a specific protein family also present?” By putting these all together, the team is beginning to discover new information about PHA production in cyanobacteria. So far this approach has helped the machine-learning team identify three PHA-production gene candidates that the team is now in the process of studying experimentally.

Dream big

When Hyatt invented celluloid in 1868 as a replacement for ivory billiard balls, he showed that a new material could be just as good, if not better, than the status quo. Celluloid was not a successful ivory replacement, but it opened the door to a new world of possibilities of polymer-based plastics, and billiard balls are now made with acrylic or plastic resins.

Traditional plastics seem today like the only material for many of life’s necessities, but history suggests the advantage of a more imaginative outlook. Through creativity and science, new materials could become competitive alternatives in the \$500 billion plastics market. Marrone, Dale, and their colleagues are making headway using microorganisms to produce muconate and PHA, but this is just the beginning, as microbe-developed polymers are on the rise throughout the research and development community.

Dale explains that her team is already moving forward to more types of plastic replacements and that she has a new project to develop absorbent biopolymers, which could mean, for example, bio-based paints and diapers. One by one, Dale hopes this work will lead to bio-based alternatives to each current plastic—ultimately leading to a healthier outlook for the future of the planet.

“This is my dream,” she says with a smile. **LDRD**

—Rebecca McDonald

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TO THE ENDS OF THE EARTH

*A special team from LOS ALAMOS manages mobile laboratories
and enables CRITICAL CLIMATE SCIENCE*

IN 1831, HIS MAJESTY'S SHIP *BEAGLE* SAILED FROM ENGLAND to circumnavigate the globe. On board were a naturalist named Darwin and a captain named FitzRoy. The broad strokes of Darwin's work are well known—finches, tortoises, natural selection. But FitzRoy's work, though also profound, is less familiar. As well as being a ship captain, FitzRoy was a scientist, like Darwin. And like Darwin, FitzRoy published a book many years later, proselytizing a disruptive new way of thinking about the natural world. He claimed that storms could be predicted.



The German icebreaker and research vessel *Polarstern* in Antarctica, 2013.

CREDIT: Alfred Wegener Institute, Stefan Hendricks. Used with permission.

FitzRoy's science was meteorology. In 1854, when his seafaring days were over, he began a weather-data collection project (which soon became the United Kingdom's Met Office). He would loan meteorological instruments to ships and coastal towns for the purpose of monitoring the weather. Using the collected data, he began making weather predictions, for which he coined the term "forecast." FitzRoy's forecasts, accurate more often than not, were transmitted by telegraph, the newest technology of the time.

Fast forward 166 years. Weather forecasting and climate research have come a long way, now involving satellites, drones, and supercomputers. But FitzRoy's essential idea—to crowdsource the collection of data by loaning equipment to users far and wide—endures. One such program is supported by a dedicated group of scientists and engineers based at

observations and inform sustainable solutions to environmental challenges. It is unrealistic, from a cost-benefit perspective, for every climate scientist to own, maintain, and operate all of the scientific instruments he or she may need. So the ARM user facility is a way for many researchers to have access to a full complement of state-of-the-art scientific instruments.

As well as several fixed-location laboratories, ARM has three mobile laboratories—suites of equipment that are built to travel. Each mobile laboratory has about 50 instruments that can take continuous measurements of clouds, aerosols, precipitation, and other meteorological variables. These facilities can also host guest instruments or operate in collaboration with experiments from other agencies, making them ideal for multi-agency research around the world. One mobile facility is on extended deployment in Alaska, but the other two are deployed to new locations every year or so, and are managed and operated by the Los Alamos Field Instrument Deployments and Operations (FIDO) team.

The FIDO team is a little like the road crew to a band—they customize, pack, ship, set up, maintain, operate, and monitor all of the ARM mobile-facility equipment for the primary investigators who lead the research. But unlike roadies they also do the equivalent of planning the tour schedule, writing some

THE ARM PROGRAM AND THE FIDO TEAM SPECIALIZE IN THE HARD-TO-REACH PARTS OF THE PLANET

Los Alamos, some of whom are presently on an Arctic expedition the likes of which would blow even FitzRoy's forward-thinking mind.

Research roadies

The U.S. Department of Energy established a user facility in 1989 that is dedicated to climate and earth-systems research. The Atmospheric Radiation Measurement (ARM) research facility is actually multiple facilities—some permanent, some mobile. Distributed among various national laboratories, the ARM facilities enable climate

of the music, and playing most of the instruments. The FIDO team helps choose which research campaigns will get to use the ARM mobile facilities. For each of the chosen campaigns, the team works with the primary investigator to devise the science plan—which instruments will be used, which measurements will be taken, and which environment-specific customizations will be needed. FIDO also helps ARM distribute the data, free of charge,

Both of the ARM mobile facilities managed by the Los Alamos FIDO team are either in, or recently returned from the Arctic. The two science campaigns they support, MOSAiC and COMBLE, aim to improve the modeling of climate processes by collecting high-quality data about specific climate phenomena.





Members of the FIDO team setting up ARM instruments at “Met City,” the MOSAiC ice-floe research station dedicated to the collection of meteorological data. In the background, left to right, are FIDO team members Dean Greenamyre, Juarez Viegas, David Chu, Steele Griffiths, and Vagner Castro. In the foreground are ARM personnel Jody Ellis, Misha Krassovski, and Matt Boyer. The RV *Polarstern*, frozen into the ice in the far background, will be home for the next two months. The ship carries a full load of staff, researchers, and additional scientific instruments.

CREDIT: Alfred Wegener Institute, Esther Horvath. Used with permission.

to scientists throughout the world. From campaign conception to closure and beyond, the FIDO team manages everything about the ARM mobile facilities. They have so far conducted over 45 field campaigns in 19 countries.

When it comes to climate data, the easy-to-reach places are fairly well represented. The ARM program and the Los Alamos FIDO team that supports it specialize in the hard-to-reach areas of the globe. Remote, desolate, and harsh places, like mountaintops, islands, deserts, and the poles, are where the FIDO team goes. Both of the ARM mobile facilities are in, or recently returned from, the far north: One has just come back from Norway, and the other is adrift somewhere in the Arctic Ocean.

MOSAIC

The most ambitious scientific Arctic expedition of all time is happening right now, and members of the FIDO team are there. It is the largest full-year Arctic research expedition—including more than 600 expeditioners, representing 60 institutions from 20 countries. Led by the Alfred Wegener Institute, Helmholtz Centre for Polar and Marine Research (Bremerhaven, Germany), and dubbed “MOSAIC,” for “the Multidisciplinary drifting Observatory for the Study of Arctic Climate,” this field campaign will gather data from October 2019 to October 2020 about how ice, atmosphere, and ocean systems interact. A paucity of year-round observations in the central Arctic has hampered thorough scientific modeling of Arctic warming processes. The goal of MOSAiC is to remedy that and enable a better understanding of the factors that make the Arctic ground zero for global climate change.

Ships crossing the Arctic Ocean typically take great pains to avoid becoming locked into the ice. But this is no typical crossing. The Research Vessel *Polarstern*, a German icebreaker, was frozen into an ice floe, intentionally, to drift with the current through the polar night and across the central Arctic Ocean. The ship is loaded with scientists and scientific instrumentation, and research stations on the floe nearby contain even more equipment. Research staff rotate in and out every two months, traveling most of the way by icebreaker, but often taking a helicopter to cover the final miles to the RV *Polarstern*.

A two-month leg on MOSAiC is really a four-month commitment—it can take a month just to get there, especially in winter, and another month to get back. FIDO team member Paul Ortega, who has just returned from a stint aboard the *Polarstern*, explains, “Just getting there on the Russian icebreaker *Kapitan Dranitsyn* was not guaranteed. We spent four weeks breaking through the ice wondering if the *Polarstern* was drifting away from us faster than we were approaching it.”

Ortega was there to support an ARM mobile facility that is being used by Matthew Shupe of the University of Colorado, who is one of MOSAiC’s co-coordinators. Shupe is collecting data on the properties of, and interactions between, clouds, solar radiation, heat fluxes, precipitation, and aerosols in the air. The fifteen or so shipbound ARM instruments include radars for characterizing clouds and precipitation, lidars for measuring air turbulence, and a suite of analytical instruments for measuring air chemistry. Additional ARM instruments for measuring precipitation, surface radiation, wind, and carbon dioxide are deployed at “Met City,” MOSAiC’s ice-floe station dedicated to meteorological data collection. (Other nearby ice-floe stations for the expedition are Ocean City, Ice City, and ROV city, the last of these being home-base for a menagerie of remotely operated vehicles).

“The Los Alamos component is by far the largest in terms of number of instruments deployed, sophistication of instrumentation, and the amount of data being collected,” says FIDO programmatic team leader Heath Powers. “Most of the ARM instruments are so sophisticated that each would ordinarily require a dedicated scientist to babysit it. But we can operate with just three team members on site at a time because of continuity of experience—our team is intimately familiar with these exact instruments because we’ve been working with them, under all kinds of conditions, for years.”

The FIDO team members are mainly scientists and engineers within the Laboratory’s Earth and Environmental Sciences Division. Though they aren’t always subject-matter experts in terms of each scientific experiment, they are unequivocally subject-matter experts in international project management and logistics, as well as experts in the operation of the instruments themselves.

“Do you know why they are called instruments, instead of machines?” asks David Chu, a FIDO operations manager recently returned from MOSAiC. “It’s because an instrument needs to be expertly tuned in order to operate correctly. Just like musical instruments, our instruments take skill and practice to operate, and they are extremely sensitive to things like vibrations and temperature changes.”

The team has to anticipate these kinds of challenges and prepare solutions well in advance of deployment. Here again the continuity of experience that comes from having a designated team allows previous

experience to help. When the FIDO team first deployed an ARM mobile laboratory to Antarctica for a 2015 campaign, it took a lot of time and effort to figure out how to prepare the instruments not just for life in Antarctica, but for life on the ship as well. The solutions developed for Antarctica helped the team plan for the MOSAiC expedition in the Arctic.

SHIPS CROSSING THE ARCTIC TYPICALLY TRY TO AVOID BECOMING LOCKED INTO THE ICE— BUT THIS IS NO TYPICAL CROSSING

For example, the FIDO team needed to install a scanning cloud radar system somewhere on the ship (this was, in fact, the first-ever deployment of a scanning cloud radar over Arctic sea ice). This is an invaluable tool for understanding clouds—specifically for filling in uncertainty in predicting cloud cover, thickness, size, and composition, which are among the largest sources of uncertainty in climate models. The instruments involved are not intended to travel; they are extremely complex and intended to sit safely and stationary on a stable surface. Furthermore, the system needs an unobstructed view of the sky, which is difficult to find on a ship because of masts, crow’s nests, and other infrastructure. The team chose a location on the very top of the ship, but the added weight of the instrument (which includes a shipping container for support) could affect the ship’s balance and handling, so the team needed to add ballast to the bottom of the ship to counteract the added weight up top.

Reinforcement had to be added to the ship itself as well, because the deck where the scanning cloud radar system was installed is located directly over the bridge, where the captain and crew spend most of their time. Anything that gets attached to the ship, whether instrumentation or reinforcement—also has to be inspected and certified by Germany’s naval architects as well as the owner, manager, and insuring agencies for the RV *Polarstern*.

In addition to installation challenges, there are also operational challenges to overcome. The ship uses radar and many radio frequencies for navigation and communication, so a lot of work went into deconfliction—the process of ensuring that the research instruments didn’t have any effects on the ship’s instruments or other researchers’ instruments, and vice versa. And all that is just to get one instrument—the scanning cloud radar system—squared away.

COMBLE

The other ARM mobile facility managed by the FIDO team was, until last month, not far from MOSAiC, in northern Norway. For four months, FIDO staff collected data on clouds and precipitation at two locations, one on the northeastern coast and another on a tiny island even further north. The campaign is called COMBLE, for Cold-air Outbreaks in the Marine Boundary Layer Experiment. A cold-air outbreak is a

SAFETY FIRST

SOME OF THE MOSAiC EXPEDITION'S
SAFETY PRECAUTIONS



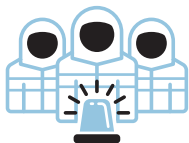
Everyone receives training for Arctic field safety (including polar bear safety and first aid), and maritime professional training (including shipboard firefighting and CPR).

A polar bear perimeter around the ship includes trip wires that automatically set off loud pyrotechnic blasts when triggered.



Onboard infrared scanners and cameras constantly monitor the horizon and ice camps to look for bears in the dark.

Daily safety meetings cover the day’s activities, hazards, and situational awareness.



Leaving the ship and traveling on ice must be done in groups; an automated system will sound an alarm if a group does not return on time.

Groups traveling large distances must carry additional communications devices and firearms for their protection.



Polar bear guards are on the ice during all working hours, and lookouts watch from strategic positions.

In between science campaigns, the ARM mobile facilities return to Los Alamos, where they are repaired, updated, customized, and tested prior to redeployment. Pictured below are FIDO team member Paul Ortega and Colorado State University aerosol chemist Jessie Creamean. (Right) A disdrometer, or precipitation gauge, sits on a tripod surrounded by a ring-shaped wind shield.



(Left) A beam-steerable radar wind profiler (gray dome with fences attached), which measures wind velocity; a Ka-band zenith radar (white drum), which probes the extent and composition of clouds directly overhead; and the inlet stack (gray tube with silver dome on top) for the Aerosol Observing System, a collection of additional instruments housed in the shipping container beneath it.

CREDIT: New Mexico images courtesy of the U.S. Department of Energy Atmospheric Radiation Measurement (ARM) user facility; photos by Anjeli Doty/LANL.

Arctic images courtesy of Alfred Wegener Institute, Esther Horvath. Used with permission.

THE DIFFERENCE BETWEEN MACHINES AND INSTRUMENTS IS THAT INSTRUMENTS NEED TUNING BY EXPERTS

high-latitude phenomenon in which cold air from the polar cap sweeps past the edge of the ice and out over open water. COMBLE is studying the dynamics and properties of clouds that are formed during cold-air outbreaks. Though smaller in scale, COMBLE's ultimate goal is the same as MOSAiC's: to improve the modeling of climate processes by collecting high-quality data about specific phenomena that presently lack high-quality data.

Prior to COMBLE, this mobile facility was in Argentina, and next it will be deployed to Houston, Texas. The other ARM mobile facility, prior to MOSAiC, was on an icebreaker in the Southern Ocean, and when it returns from MOSAiC it will go to Crested Butte, Colorado. In between campaigns, the ARM mobile laboratories return to Los Alamos to be spruced up—damage gets repaired, parts get replaced, software gets updated. Then the team members prepare the instruments and themselves for their next deployment.

The long arm of ARM

In his groundbreaking 1863 book, *A Manual of Practical Meteorology*, FitzRoy wrote, "It seems advisable to consider meteorologic conditions of our world as if we looked down on it from without. When a terrestrial globe is before the eye, relative sizes, spaces, distances, extensions in area, and depths, are less inaccurately viewed."

The ARM program, with the support of teams like the Los Alamos FIDO team, is working to do just that: to improve humanity's understanding of Earth's climate as a whole by helping

scientists gather the information they need from the places they need it—from pole to pole and on every continent in the world.

FitzRoy circumnavigated the globe, watching the weather and studying the sea. Now the FIDO team follows in his wake, traveling to the ends of the earth and back again, taking ARM's modern mobile laboratories to the places where they are needed the most. The ships are bigger and the instruments fancier, but what drives them is unchanged: the eternal, elemental need to know.


—Eleanor Hutterer

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High-energy protons could provide better imaging, better targeting, and better treatment.

CANCER IN THE CROSSHAIRS

THE RELATIONSHIP BETWEEN CANCER AND RADIATION IS... complicated. Radiation can definitely cause cancer. But it can also cure cancer. And when used in medical imaging, radiation can help diagnose cancer.

In medicine, “radiation” is a catch-all term used for several different types of electromagnetic waves (e.g., x-rays, gamma rays) or subatomic particles (e.g., protons, positrons) that are used for imaging or therapy. Of the particles presently used for cancer treatment, protons are at the cutting edge, and researchers at Los Alamos have recently reported several discoveries that could make proton-based cancer diagnosis and treatment even better.

What they’ve demonstrated amounts to improved imaging accuracy, tighter tumor targeting, and even the potential for earlier diagnosis. Los Alamos medical physicist Matt Freeman puts it succinctly, saying, “Our goal is to apply imaging techniques to make therapy better. This is where our work lies, at the place where imaging and therapy meet.”

Better targeting

The Los Alamos Neutron Science Center, or LANSCE, is home to a particle accelerator that produces protons with energies up to 800 megaelectronvolts (MeV). LANSCE has a sister facility of sorts in the GSI Helmholtz Centre for Heavy Ion Research, in Darmstadt, Germany. Scientists from the two centers collaborate frequently, and it was during a 2009 visit to Darmstadt that Los Alamos physicist Frank Merrill and his German colleagues had an idea while brainstorming over a beer. Merrill was interested in new applications for LANSCE’s high-energy protons, and the Germans were interested in new ways of treating tumors while they are still very small. As the scientists conversed, they

realized their two interests just may be the answers to each other’s questions. High-energy protons might *be* the way to treat very small tumors. Prost! (German for “cheers!”)

If an animal cell’s DNA is damaged in such a way that the cell loses its ability to control its own life cycle and begins to divide rampantly, the result is cancer. But if a cancer cell’s DNA is damaged such that the cell can’t successfully divide at all, then the cell dies. Modern medicine has devised multiple ways to target cancer cells with DNA-damaging radiation. Most common is the injection or implantation of a radioactive substance or the transmission of a beam of radiation into the body from an outside source. With each of these methods, the goal is to do more damage to the cancer cells than to neighboring, non-cancer cells. It is in this way that protons are just about perfect.

Other types of therapeutic beam radiation pass all the way through a human body, potentially damaging everything on their path to and from the tumor. But protons only travel a certain distance, based on their starting energy; they gradually lose energy along the way, then stop and dump their remaining energy rapidly as they come to rest. The energy the protons lose on the way in does cause some unwanted damage, but most of the damage is concentrated onto the tumor. As long as the proton energy is suitably controlled, there is no exit path and therefore no exit-path damage.

Because they are positively charged, protons scatter as they pass through an object—they get pushed around a little bit by each atom they encounter, being drawn toward negative charges and repelled by positive ones. This scatter is largest at the end of the trajectory, causing the energetic protons to laterally spread into the immediately surrounding tissue, which, if the aim is true, should be tumor tissue.

Different materials have different stopping power—that is, how much energy they absorb from a proton per unit volume of material. Increasing the proton beam's energy increases the beam's penetration range. When the stopping power is known, the penetration depth can be precisely tuned by controlling the energy of the beam. For example, 230-MeV protons have a penetration range of 30 centimeters (cm) in soft human tissue. Protons for cancer therapy typically range from 230 to 330 MeV and are commonly produced by a cyclotron—a particle accelerator that is compact enough for clinical spaces.

Although it's ideal for protecting tissue from exit-path radiation, current proton therapy can't target tumors smaller than about a centimeter in diameter. This is because of the way the protons spread laterally into the tissue when they come to a stop. Protons that start at 230 MeV dump their energy into about 1.5 cm of surrounding tissue. If the tumor is much smaller than that, too much healthy tissue gets the dose.

Merrill and his German colleagues realized that high-energy protons could theoretically target tumors as small as 1.0 millimeter (mm). High-energy protons, like the ones at LANSCE, actually do pass all the way through the patient with relatively little scatter, taking most of their energy with them. This means minimal lateral spread, which means tighter tumor margins, which means less risk to surrounding tissue, which means smaller tumor targets. It would be like painting with a 0.3-cm paintbrush, compared to the current standard 1.5-cm paintbrush.

But the reduction in tumor size comes at a cost. Lower-energy protons don't have exit paths, but high-energy protons do, which increases the collateral damage. Additionally, because the bulk of the protons' energy remains with the protons through the tumor and out the other side, there needs to be some way of boosting the energy deposited in the tumor, relative to the entry and exit paths. The way to do this is to use a highly controlled beam of high-energy protons and rotate it around the patient during treatment, irradiating the tumor from 360 degrees. This dramatically dilutes the dose to entry- and exit-path tissues, while maximizing the dose to tumor tissue.

"Treating tumors with high-energy protons is a good idea, but it's still theoretical, and Los Alamos isn't exactly a cancer-treatment facility," explains Laboratory physicist Michelle Espy, who works with Freeman and Merrill. "But we're trying to think about what the clinics will want to be doing ten years from now. We're developing the science now so that it's ready when the clinicians need it."

When the accelerators in the clinical instruments are able to give more energy, the beams will be able to treat smaller tumors. And as the target sizes decrease, the need to see them precisely will increase. So, Freeman, Merrill, and Espy, along with their colleague Dale Tupa and students Ethan Aulwes, Rachel Sidebottom, and Brittany Broder have been working on that too.

Better imaging

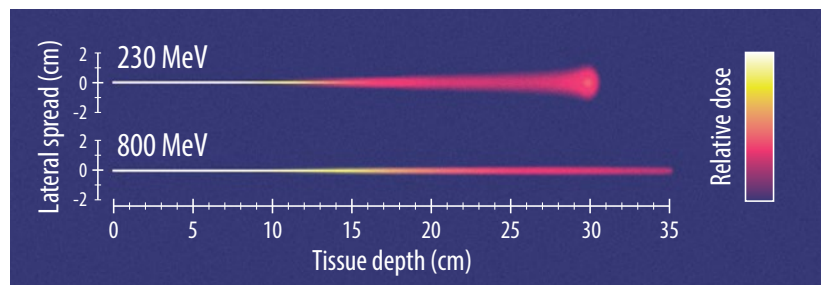
Contemporary proton therapy is becoming more and more accessible, but concomitant improvements in imaging are needed. Treatment planning relies on careful imaging and measuring of the tumor target, to make a 3D map of intended hits and misses.

But this is often done on one day, while the actual treatment is done over the course of weeks. Human bodies are squishy—they swell, shrink, and shift from one day to the next. If a target is very close to something crucial, and things have moved around a bit, the therapy could wind up doing more harm than good.

The current state of the art for precise proton-beam targeting is to use x-ray imaging during, as well as before, the proton therapy. This gets around some of the squishy issues, but the x-rays are oriented at different angles to the proton beam, so even though it's real-time, it's still not a perfect view. The ideal would be to see the target as the therapy protons see it, from a "beam's-eye view."

Our work lies at the place where imaging and therapy meet.

Freeman explains, "Beam's-eye-view radiography can help prepare for a patient's treatment because it provides a better map to more accurately constrain the dose, which helps spare nearby tissues. It can



also be used to guide a dose in real time and correct for day-to-day or even minute-to-minute changes in patient anatomy."

Conveniently, high-energy protons like the ones that could safely target mm-sized tumors can also be used to visualize the internal structures of things. The technology, called proton radiography, was discovered in the 1970s and has been developed and perfected at LANSCE for national security applications. Proton radiography, or pRad for short, produces an image of an object's density by shooting protons through the object and then mapping the transmission of the protons to density variations in the material.

Because the protons scatter as they pass through the object being imaged, without

Tissue penetration power and dose deposition of high-energy protons (800 MeV) compared to what is presently used in proton-beam therapy (230 MeV). At 30 cm, the 230-MeV protons stop and dump their energy into about 1.5 cm of surrounding tissue. By contrast, the 800-MeV beam doesn't stop at all and spreads minimally (0.3 cm) as it travels through the tissue.

some kind of correction, the resulting image would be blurry. The thicker the object, the more scatter and the blurrier the image. And although the scatter is caused by the protons' positive charge, so too is the solution.

"It's just magnets!" exclaims Espy. "Because protons are charged, we can take all the scatter and bend it back using magnets to focus it, and we actually wind up with a very good image."

Magnetic focusing lenses cancel the would-be blur by focusing the protons onto a specific plane, similar to how optical lenses focus light onto a specific plane (e.g., a screen, a piece of film, or a retina). A series of magnetic quadrupoles surround the proton beam in a perpendicular orientation, each with two north and two south poles in alternating orientations. The magnetic field is zero at the center of the beam line and gets stronger towards the periphery, where more powerful steering is required to refocus the protons. The most highly scattered protons create blurring in the final image, so these get removed at an earlier collimation point, while the rest of the protons continue on to converge on the image plane.

Proton radiography at Los Alamos is definitely not new—in fact, it's a Laboratory specialty. But the idea of using pRad in tandem with high-energy proton-beam therapy for cancer treatment

is new. And although the Laboratory isn't the place to implement clinical beam's-eye-view radiography, it is certainly the place to develop the science.

"We are evaluating lens-based pRad, of the sort done regularly at LANSCE, for guiding proton-beam therapy," explains Freeman, "and we're sharing our findings with the medical imaging and radiotherapy communities in the hope that they'll invest in the needed infrastructure. When they do, they'll simultaneously unlock new treatment and imaging capabilities."

If combined with high-energy proton therapy, beam's-eye-view pRad would not increase the overall radiation that a patient receives, and might even decrease it, because imaging and treatment could both be achieved with a single beam. But it doesn't have to be combined with new therapy technology—beam's-eye-view pRad could benefit proton therapy now. It's actually better at pinpointing the stopping power than x-ray radiography is, so it would improve dose calculation and mapping.

"This is certainly something clinics could implement," says Espy. "Once you have the protons—which any proton-therapy clinic already does—you can add the optics to the existing system. Imaging would be nearly instantaneous."

Seeing tiny tumors from a beam's-eye view helps with accuracy, but the densities of tumors and healthy tissue are similar, and it can be hard to distinguish the two using a density-based imaging technique. So the team has been working on that too.

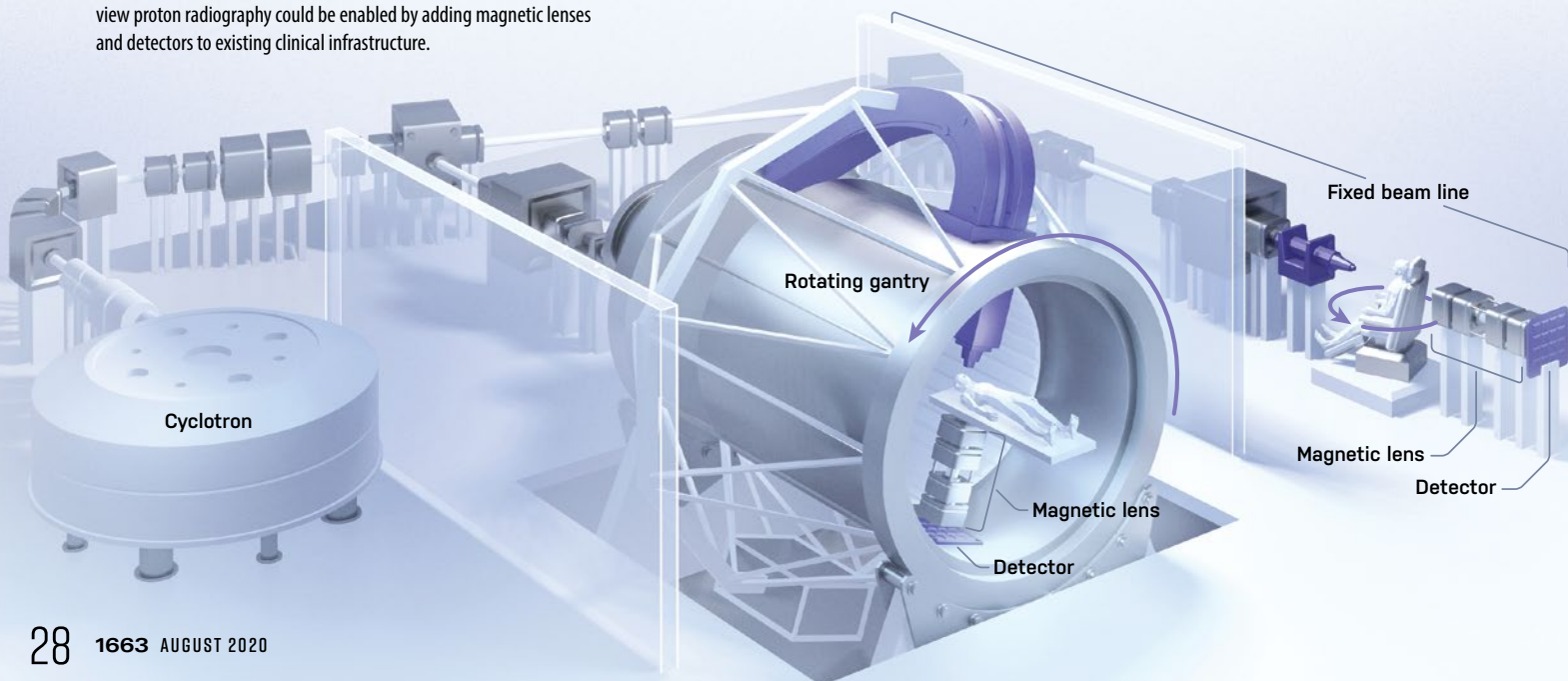
Even better imaging, and a capability too

"The challenge of seeing a tumor is just that," says Merrill. "It's something that will keep scientists busy for a while."

Because tumors and healthy tissue look similar to pRad, there has to be a way to tell them apart. There are two general approaches for this: either magnify their differences, or increase the sensitivity of the tool. In pursuit of beam's-eye-view pRad, the Los Alamos team has done both.

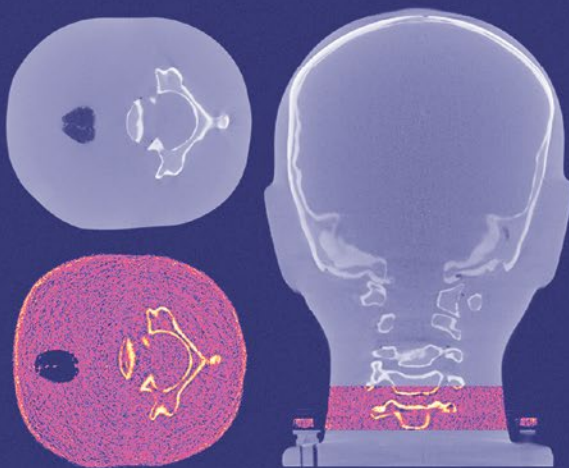
Initially the scientists went down the path of magnifying differences. One difference between healthy cells and cancerous cells is the number of certain receptor proteins on their surfaces—often cancer cells have more. Gold nanoparticles can be tethered

Proton therapy for treating cancer is typically done in one of two ways: either the patient lies immobile while the gantry-mounted proton beam rotates (center), or the proton beam is immobile while the patient is re-positioned (right). In either configuration, instantaneous beam's-eye-view proton radiography could be enabled by adding magnetic lenses and detectors to existing clinical infrastructure.

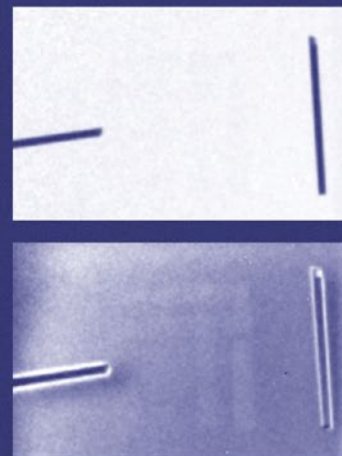


An x-ray radiograph (top left) and a proton radiograph (bottom left) show a cross section through the neck of an artificial pediatric head, designed for medical imaging. (Right) A composite image.

Although the proton radiograph portion is noisier, the anatomy is still easily identified with 800-MeV protons. With beam's-eye-view imaging, the proton beam that produces the image would also deliver the treatment dose, improving accuracy and reducing radiologic exposure.



Even state-of-the-art collimation for proton radiography of thin systems (top) cannot resolve, to any useful degree, a basket weave pattern in gold leaf. But dark-field proton radiography (bottom) clearly shows the basket-weave pattern by enhancing contrast between the layers. (Perpendicular black bars at left and right are for image orientation.)



to molecules that specifically bind these proteins, so that when those molecules are introduced into the body, the tumor winds up effectively covered in gold. Gold is a good contrast agent because it's not very toxic to cells and it decreases transmission relative to unlabeled tissue. Target cancer cells can take up about 100,000 nanoparticles per cell, which makes 1-mm tumors plainly visible to pRad.

But nanoparticle enhancement of contrast is difficult to do, and it depends on the tissue type and tumor location, so it isn't always feasible. The team also wanted to increase the sensitivity of the imaging tool. "Dark-field microscopy" is an optical method

gold leaves, arranged in a basket-weave pattern, way better than they had dared to hope. Prost again!

To the scientists, this is the most exciting of their recent discoveries. Whereas high-energy proton-beam therapy and beam's-eye-view pRad are important proofs of principle, they are trees that will bear their fruit primarily outside of the Laboratory. But dark-field pRad represents a new institutional capability for Los Alamos. And it's done, it's here, it's ready to use.

Because it's so new, only just having been proven for the first time, the team is confident that the technique can be made to work even better. It will mainly be useful for visualizing very thin

Dark-field proton radiography is here. Now. It's a Lab capability that's ready to use.

of enhancing the contrast between two difficult-to-distinguish things by imaging with scattered particles (photons for light microscopy, electrons for electron microscopy), rather than unscattered particles. Dark-field imaging thus yields a plain black image when nothing is there. Dark-field pRad had previously been theorized but never demonstrated. The method would be very sensitive to minute differences, which is why the team wanted to try it.

The scientists were testing different collimation schemes for beam's-eye-view pRad when they realized they were perfectly positioned to try and prove dark-field pRad. Prior attempts to demonstrate dark-field pRad had only used one collimator, but the trick, it turned out, was to use two collimators: the standard one to exclude the most highly scattered protons, which create blur, and another to exclude the *least* scattered protons. These bring noise to the image and carry comparatively little radiographic information, so excluding them increased the signal-to-noise ratio, which improved the image dramatically.

The week before Christmas, 2019, the team was working to squeeze in one more run on LANSCE's proton beam before leaving for the holidays. They were attempting to do dark-field pRad on a few pieces of gold leaf—less than a millionth of a meter thick and designed by Tupa to simulate a gold-labeled tumor. And lo and behold, it worked. They could see the millionth-of-a-meter

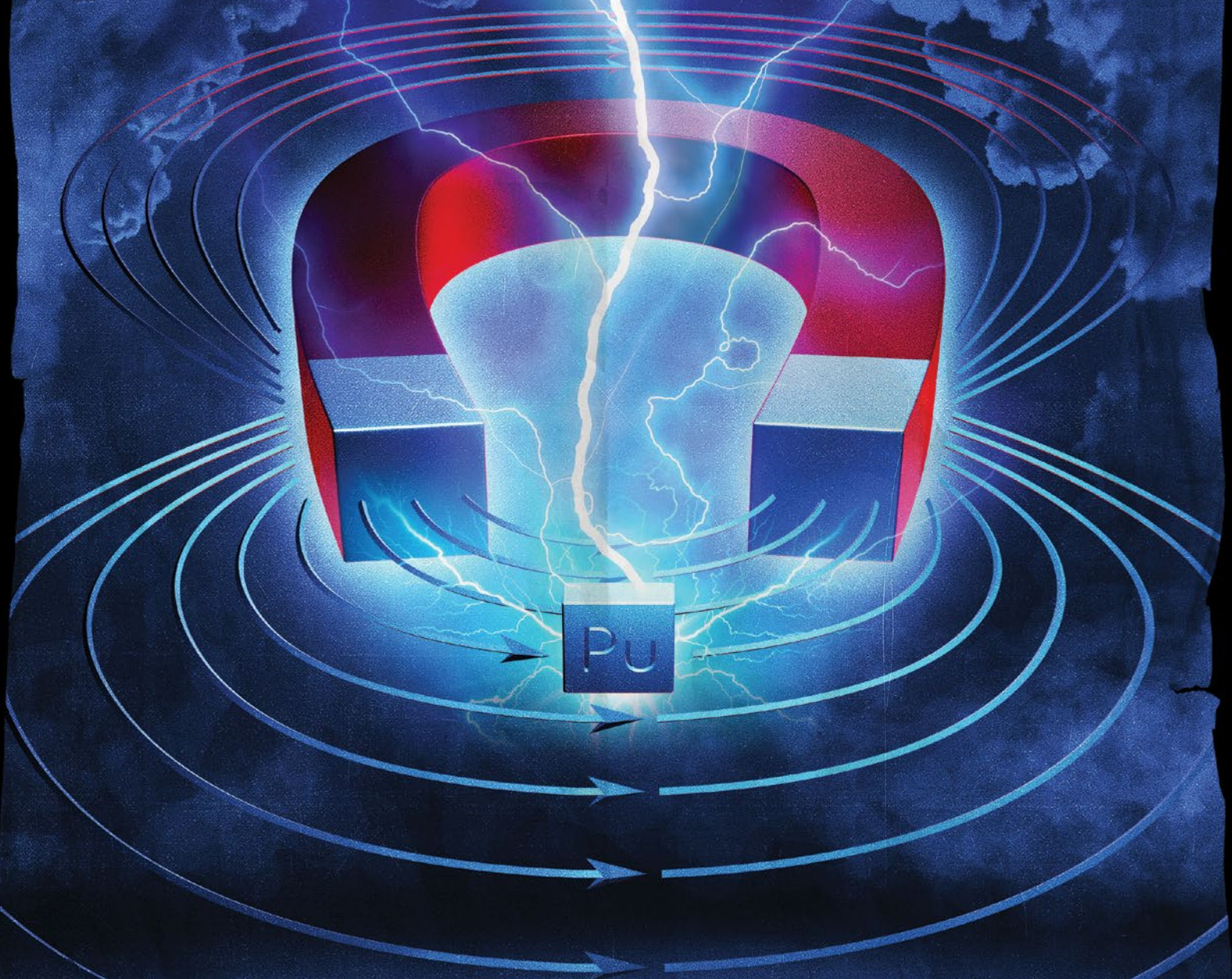
things and very subtle differences. Mission-centric applications include visualizing the evolution of high-explosive detonation products, the breakup of ejecta material, or the mixing of certain gases after being shocked.

LANSCE is home to a pRad user facility, where scientists from around the world can come do pRad experiments. Now dark-field pRad will be available to those users too. Dark-field pRad is a lasting legacy for pRad, which itself is a lasting legacy for Los Alamos.

These scientists have moved science forward on two fronts. First, they've fleshed out a three-pronged improvement to cancer treatment: High-energy proton-beam therapy could improve cancer prognoses by targeting tumors when they are still only millimeters across; beam's-eye-view pRad can bring higher accuracy to treatment dose calculation and dose delivery; and dark-field pRad can aid in both imaging and treatment by better distinguishing tumors from healthy tissues. Second, and not to be outdone, they've developed an entirely new capability for the Laboratory and the proton radiography community at large. Prost, indeed! **LDRD**

—Eleanor Hutterer

MAGNETOSTRICTION



THE DISSONANCE OF VOLUME TOUR
"HEAT IT UP TO BRING IT DOWN"

FIRST-EVER MEASUREMENT of temperature-activated electron reconfiguration—and decreasing volume—in the **WORLD'S STRANGEST METAL**

PLUTONIUM IS KNOWN FAR AND WIDE for its nuclear properties. But in certain circles, it's also known for its material properties. The manmade metal comes in *six* distinct solid crystalline structures spanning a wide array of chemical properties and a stupendous range in volume. At one end of the spectrum, alpha plutonium (α -Pu) is brittle and extremely dense; at the other, the same mass of delta plutonium (δ -Pu) is much softer and more ductile, and it takes up an astonishing 25 percent more space.

Equally confounding, these changes in structure and behavior, which run from α through δ and beyond as temperatures rise, reverse direction along the way. Up to about 320 °C, the onset of δ -Pu, volume increases with increasing temperature. This

explain its anomalous volume behavior. The price for that access is an enormous magnetic field.

“It would be great if everyday magnetic fields could be used for magnetostriction, like ‘a little magnetism goes a long way,’” says Harrison. “But it’s actually the opposite. You need a tremendous magnetic field to see tiny volume changes, even though changes thousands of times larger are easily brought about by heating.”

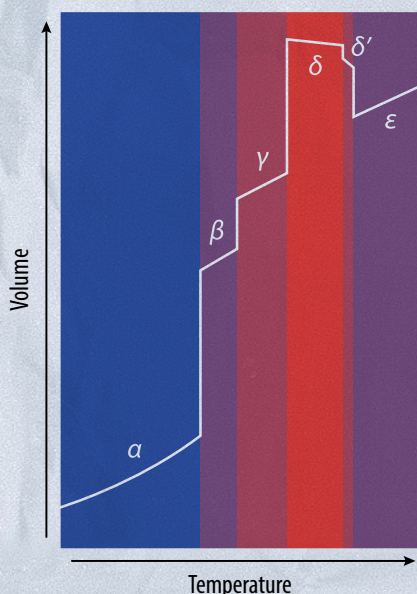
The research team used magnetic fields ranging up to a colossal

IN EFFECT, THE PLUTONIUM DEMONSTRATED **NEW WAYS TO ABSORB ENERGY WITHOUT GETTING HOTTER**

is a normal material behavior known as thermal expansion: higher temperature means stronger vibrations across the lattice of atoms that make up the material, and those vibrations are accommodated by a modest expansion in size. For the next 165 degrees, however, the volume decreases; this is not normal. It is a peculiarity of δ -Pu (and the next state after that as well) and somehow works in opposition to the increasing lattice vibrations. (Thereafter, plutonium enters its sixth and final solid state, in which volume returns to its initial dynamic, increasing with temperature.)

Explaining the 25 percent volume disparity and its reversal in direction with anything more concrete than educated speculation has been all but impossible for as long as the metal has existed. Recently, however, Los Alamos physicist Neil Harrison and materials scientist Paul Tobash and their colleagues found fresh inspiration to attempt a new kind of experiment on plutonium. Magnetostriction, as it is known, measures volume changes occurring in response to a strong magnetic field as a tiny fraction of the atoms of the bulk material magnetize and align with the external field. Unlike elevated temperatures, magnetostriction almost exclusively affects the configuration of electrons in the material, not the atomic lattice vibrations. For that reason, it accesses a separate, electronic aspect of the properties of plutonium metal—one that might

15 teslas. (The earth’s magnetic field is 35–65 *millionths* of a tesla.) Even so, the plutonium stretched by only about one millionth of its original length on a side. An extremely powerful (but nondestructive) magnetic field source is

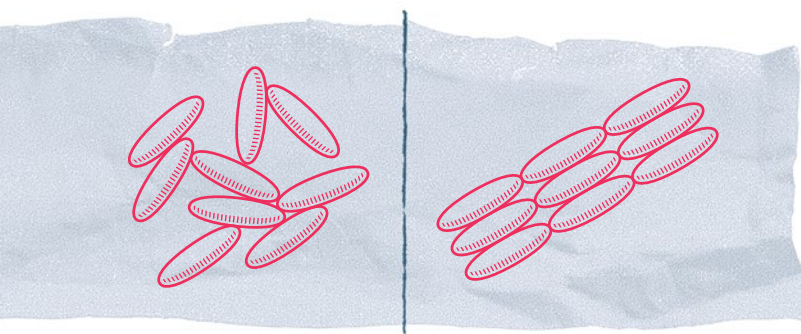


Solid plutonium metal exists in six distinct crystal structures. From absolute zero to somewhat above the boiling point of water, the first of these, α -plutonium, or α -Pu, exists. It, as well as the next two structures, β -Pu and γ -Pu, and later ϵ -Pu, obeys standard thermal expansion: higher temperatures require the metal to swell to greater volumes to accommodate increased atomic-lattice vibrations. However, anomalously for δ -Pu (and its successor, δ' -Pu), which exists naturally at temperatures several hundred degrees above α -Pu, the behavior reverses, with the graph sloping downward: the metal shrinks when further heated. Evidently, for δ -Pu, the metal is able to absorb heat energy in some manner other than increased vibrations in the atomic lattice.

needed to produce the expansion, and an extremely sensitive optical measurement apparatus is needed to notice it. But with access to the National High Magnetic Field Laboratory and Los Alamos capabilities in plutonium sample preparation, optical Bragg reflection, and cryogenic temperature regulation, the researchers were able to isolate and quantify the effect. And the result was every bit as illuminating as they hoped it would be.

Electronic entropy

As had been long suspected, the magnetostriction measurement confirmed an electronic effect that operates alongside normal thermal expansion. At just a hair above absolute zero, and therefore firmly in plutonium's ground-state configuration, sweeping the magnetic field up to 15 teslas didn't do anything; the electron configuration was essentially nonmagnetic. But starting 50 degrees hotter, the electronic configuration began to change; the atoms of plutonium became faintly magnetizable and the applied field caused the metal to expand. Then, nearing room temperature, the electrons began to reorganize again. The plutonium became more magnetizable but reversed its response to the applied magnetic field and got smaller—at long last demonstrating the origin, electronic in nature, of plutonium's anomalous volume-reversing behavior.



Magnetostriction occurs when a material is subjected to a large external magnetic field. Microscopic magnetic regions within the material undergo a reorientation, stretching or squeezing the overall material along different axes.

What exactly are the electrons doing differently? Well, they could be doing a lot of things. Unlike the first 88 elements on the periodic table (which have up to 88 electrons), ground-state plutonium, element 94, has six electrons in the 5f

orbitals. Such 5f electrons are extremely complicated. The nature of the orbitals themselves and their large distance from the atomic nucleus give 5f electrons a lot of freedom to interact with other electrons while remaining localized to the same atom or becoming itinerant, roaming from one atom to the next across the metal (and interacting with other itinerant electrons). That makes plutonium's electronic configuration far more complicated than that of an element without 5f electrons. But even among the handful of elements with 5f electrons, plutonium is arguably the most difficult to understand.

Take americium, for example, plutonium's next-door neighbor on the periodic table. It has seven 5f electrons; any or all of these have the potential to be localized (confined within atomic orbitals) or itinerant. In each case, there is an energy-minimizing configuration that corresponds to a distinct volume, and in americium the energy is always minimized when six electrons are localized.

NOTHING LIKE THIS OCCURS IN ORDINARY METALS

However, for plutonium's six (total) 5f electrons, it happens that for most of the energy-minimizing configurations, many different volume states share nearly the same energy, making it very difficult to determine which configurations are most relevant. Fortunately, the volume for each energy-minimizing configuration always gets larger when an additional 5f electron becomes localized. Therefore, Harrison and Tobash were able to pick up on all the measurable energy differences between plutonium's electronic configurations accessed with increasing temperature, allowing them to go from the ground state to expansion and then contraction.

In thermodynamic parlance, the experiment had isolated the metal's electronic entropy: increasing energy (whether by magnetism or by heating) brings about "disorder" in the form of a proliferation of electron states within the atoms, rather than just amplifying lattice vibrations. In effect, solid plutonium was shown to have new ways to absorb energy without getting hotter. And in the case of δ -Pu, absorbing that additional energy involves reconfiguring the electrons in such a way that the atoms pack together much more tightly, greatly overpowering the normal effect from lattice vibrations.

"Nothing like this occurs in ordinary metals," says Harrison. "Minor temperature changes access whole new electronic states in a way that no prior theory of plutonium could explain. And by observing a much smaller effect in response to an external magnetic field, we were finally able to show what's happening."

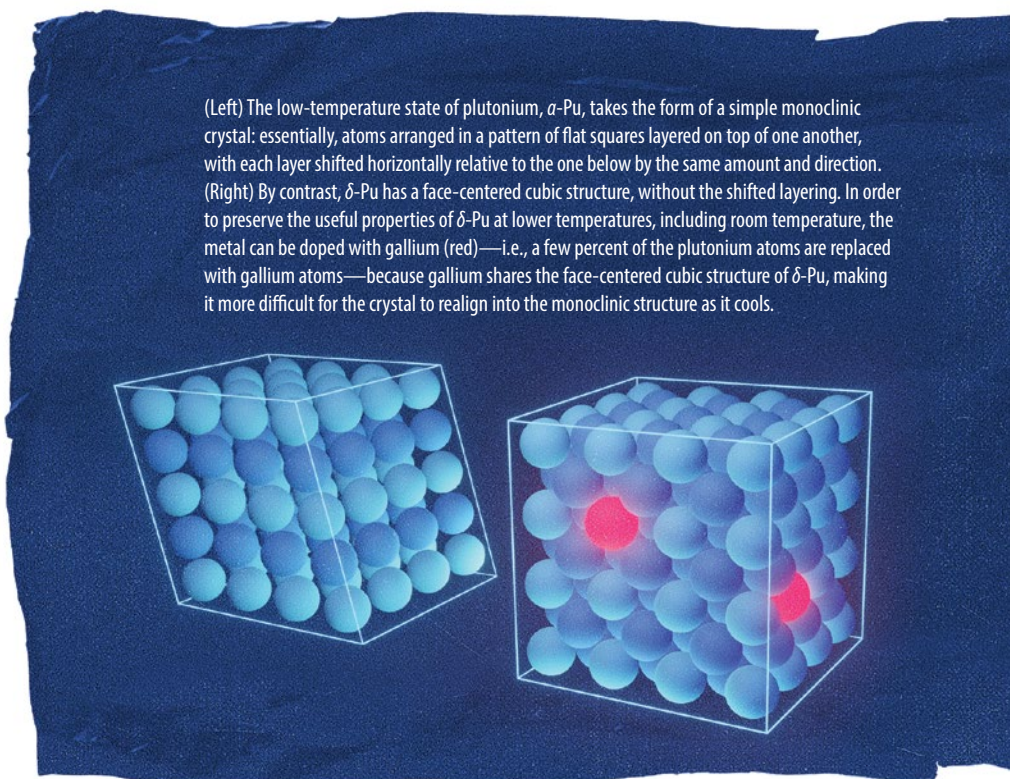
Get real

From a theoretical point of view, the magnetostriction results are a godsend. And for Tobash, who prepared the plutonium samples for the experiment, this discovery is just the beginning.

"We started with new, high-purity plutonium samples," he says. "But most of the time in real life, plutonium is neither newly manufactured nor pure." Plutonium used for real-world applications is generally doped with trace amounts of other materials. Gallium, for example, is known to stabilize δ -Pu so

that it can exist at room temperature, where pure plutonium would naturally assume the α -Pu state. Of course, one might be tempted to just avoid the mood swings of δ -Pu and be content to work with α -Pu instead, but it turns out that δ -Pu is much more useful. Not only is it softer and therefore more shapeable, but it's also less oxidizing and more stable, both chemically and mechanically. Therefore, it is standard practice to lock the δ -Pu crystal structure into place, even at room temperature. Gallium can do that because it forms bonds with the same crystal structure as δ -Pu; the α -Pu lattice, on the other hand, can't accommodate gallium quite so easily.

So Harrison, Tobash, and their collaborators performed the magnetostriction measurement with various levels of gallium doping. They found that increasing gallium concentrations corresponded to the signature δ -Pu electronic volume reversal becoming smaller than that in pure δ -Pu. Reassuringly, this is a reasonable result; replacing plutonium atoms with gallium, which has no $5f$ electrons, should tend to suppress plutonium's distinctive behavior.



(Left) The low-temperature state of plutonium, α -Pu, takes the form of a simple monoclinic crystal: essentially, atoms arranged in a pattern of flat squares layered on top of one another, with each layer shifted horizontally relative to the one below by the same amount and direction. (Right) By contrast, δ -Pu has a face-centered cubic structure, without the shifted layering. In order to preserve the useful properties of δ -Pu at lower temperatures, including room temperature, the metal can be doped with gallium (red)—i.e., a few percent of the plutonium atoms are replaced with gallium atoms—because gallium shares the face-centered cubic structure of δ -Pu, making it more difficult for the crystal to realign into the monoclinic structure as it cools.

ANYTHING MORE THAN EDUCATED SPECULATION HAS BEEN ALL BUT IMPOSSIBLE FOR AS LONG AS THE METAL HAS EXISTED

Apart from being doped, the other key aspect of real-world plutonium is that it often sits for long periods of time, such as inside a warhead at a military installation. Because of its radioactivity, high-energy particles are constantly streaming through it, creating more and more defects in its atomic structure over time. Los Alamos conducts a great deal of research on this effect in order to assess the safety, effectiveness, and reliability of aging nuclear weapons. The magnetostriction measurement and its implications for plutonium's electronic entropy provide an important basis for developing a more accurate understanding of the aging weapons in the nation's stockpile.

"Having conducted the magnetostriction experiment on newly synthesized plutonium samples, we now have a much-needed baseline," says Tobash. "From a practical perspective, the next step will be to try it on aged material, since that will add a bit more complexity with additional variables to sort out. We're planning those experiments now."

From a less purely practical perspective, another next step might be to adapt the plutonium magnetostriction results to advance scientists' theoretical understanding of its electronic properties.

"We all tend to think of plutonium in terms of the nuclear properties that make it dangerous—and no question, it certainly is that," says Harrison. "But it's also something else. From a chemistry standpoint, it is arguably the most complicated element

known. And that means that when it comes to difficult, important concepts like electronic entropy, which barely even show up in the practical applications of plutonium today, it can lead us to the scientific and technological advances of tomorrow." **LDRD**

—Craig Tyler

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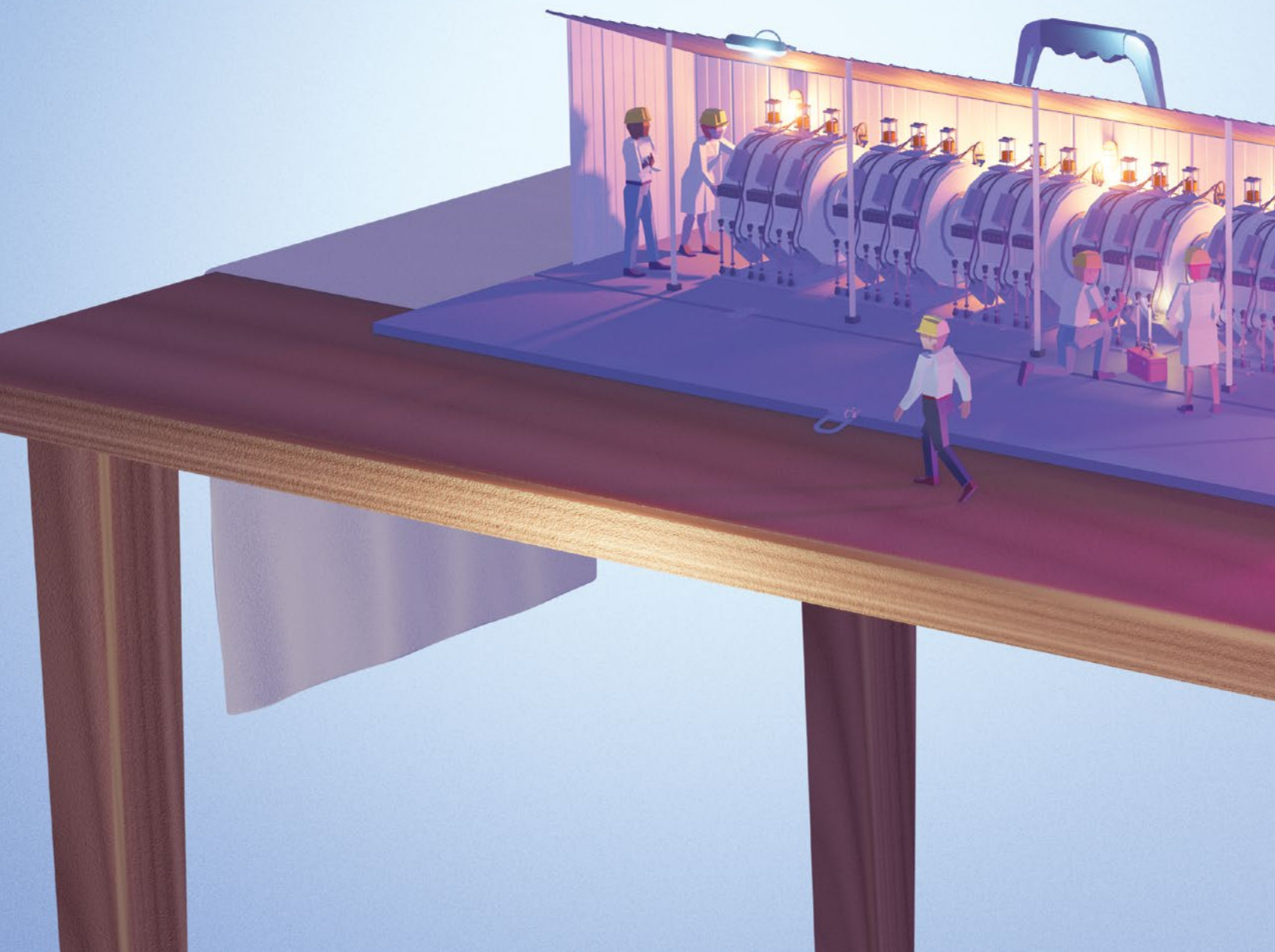
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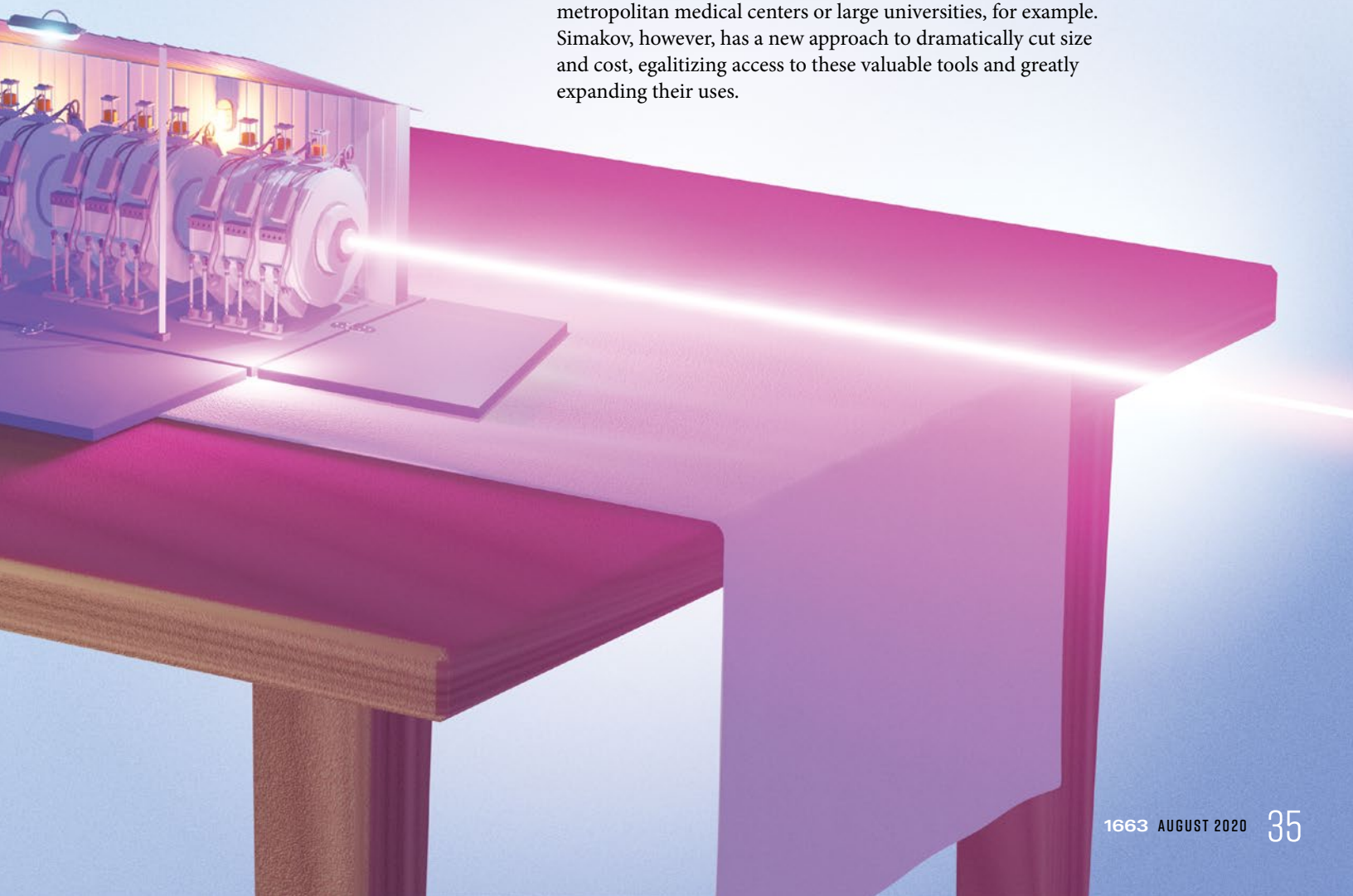


Multiple innovations enable
portable particle accelerators
for an extensive array of uses.

“WE TEND TO THINK OF PARTICLE ACCELERATORS as these enormous facilities that take decades to build and are only used for research at the very edge of known physics,” says Los Alamos physicist Evgenya Simakov. “What people don’t realize is that smaller, lower-energy particle accelerators are needed all the time—for cancer treatments and medical sterilization, security screening and defense applications, and research into new materials, biological processes, and much more.

“These smaller accelerators exist,” she clarifies. “They’re just not small enough.”

Typically the size of a small room, the accelerators in question are extremely specialized and therefore expensive. As a result, their availability is limited. Often, they are only found at major metropolitan medical centers or large universities, for example. Simakov, however, has a new approach to dramatically cut size and cost, egalitizing access to these valuable tools and greatly expanding their uses.



For example, a small accelerator can be used to sterilize foods, similar to the pasteurization of milk: killing any bacteria and parasites but leaving the food itself unharmed. This could permanently eliminate most types of food poisoning and corresponding food product recalls, such as from *E. coli* in romaine lettuce. As things stand now, the scale of such an operation makes it thoroughly cost-prohibitive in most cases. Particle accelerators would be needed all over the place: at farms, distribution centers, grocery stores, and restaurants.

Simakov thinks, why not?

To build a beam

The basic premise for a small accelerator (small compared to the likes of Fermilab or CERN, say) goes like this: a stream of particles—electrons, in Simakov's case—are pushed by an intense electromagnetic wave in a specialized conduit called a waveguide. The waveguide is what it sounds like; it's a structure designed to channel waves. One familiar type is a fiber-optic cable, made from a type of dielectric plastic with optical properties that keep visible and infrared light trapped inside. Thus, the light travels down the cable, reflecting back into the plastic whenever it bumps against the side of the fiber, rather than leaking out.

But for an accelerator, the waveguide is not such a simple matter. For one thing, the light must drive the electron beam, meaning that both the light and the electrons must occupy the same channel. Light can propagate through optical fiber, but electrons can't; they must be accelerated in a vacuum. Therefore, the waveguide has to be inverted: there must be an empty channel through the dielectric medium, with both the light waves and electrons confined within that empty region. That much is fairly straightforward to implement. However, there is another, more vexing constraint.

An electromagnetic wave carries oscillating electric and magnetic fields, the electric field being the one that a particle accelerator uses to accelerate its particles. As the light wave zigzags its way down the waveguide channel, its electric field points along various diagonals, which can be broken into lengthwise, up-down, and sideways components; the lengthwise component, directed through the channel,

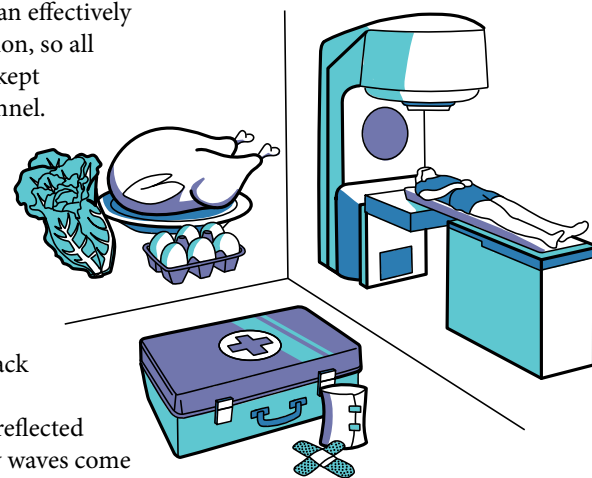
can usefully accelerate electrons. However, most optical fibers guide (reflect) waves with the opposite orientation: electric fields oscillating perpendicular to the channel only, with no lengthwise component. These are called transverse-electric, or TE, waves, as their electric fields contain no component directed along the waves' direction of motion, but rather across it. Those with the forward-backward orientation suitable for accelerating particles, called transverse-magnetic, or TM, waves, are only confined in a special kind of fiber, called a photonic band gap (PBG) waveguide. (See diagram on page 39.)

But even with a PBG waveguide—suitably hollowed to accommodate a colinear electron beam, of course—there's another problem: Because the electric fields are oscillating as waves, their lengthwise components alternately push and pull on electrons. To make an accelerator, the electrons must be fired off in precisely-timed bunches that only appear in the electric field zones that push, not pull. That in turn means the speed at which the laser's wave pattern, or phase, works its way down the length of the waveguide must be tailored to match the speed of the electrons—that is, with the laser light's phase traveling slower than the light itself. That way, the wave phase pattern and the electrons travel together: electrons enter a “push phase” and stay with it all the way down the accelerator channel. Thus, the waveguide needs to reflect not just TM waves, but TM waves with the proper phase velocity. Ordinary PBG fiber material doesn't accomplish this.

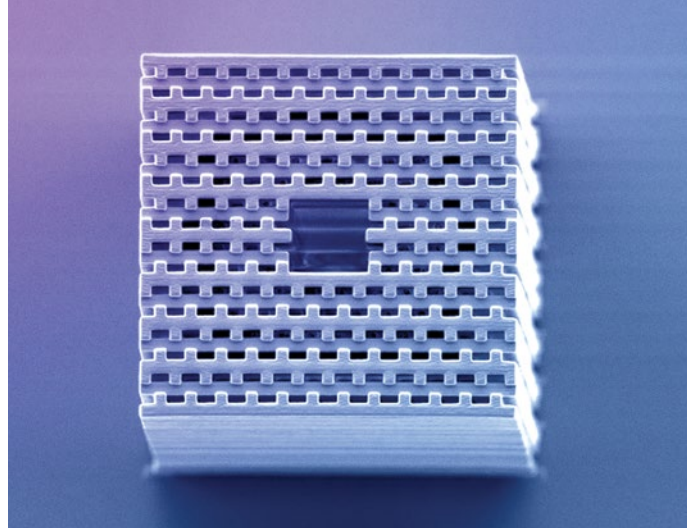
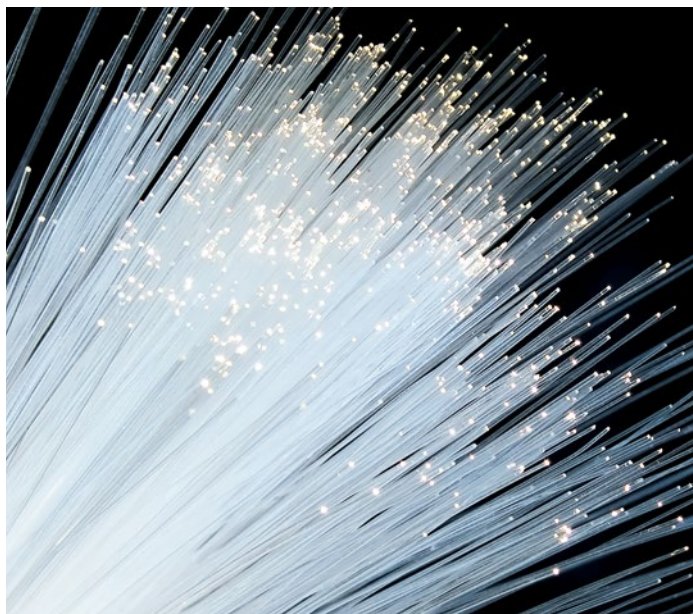
Until now, solving this problem has required a fairly serious concession: using microwaves instead of infrared or visible light. With microwaves, conducting waveguides—hollow metal ducts, essentially—will do the trick. The oscillation frequency for microwaves is slow enough that electrons in conductors are able to keep up and jiggle back and forth at the same frequency; this produces an effectively perfect reflection, so all the waves are kept inside the channel.

The interior metal walls of a microwave oven, for example, reliably reflect outbound microwaves back into the food.

But easily reflected low-frequency waves come at a cost. Microwaves have much larger wavelengths (centimeters or meters) than infrared (microns, or millionths of a meter) or visible light (fractions of a micron). To produce and channel such large waves, the waveguides and other necessary hardware, including the microwave source, must be sized in multiples of the wavelength, ranging from 10 centimeters to several meters. In large part, this is what



Some **medical applications** for compact particle accelerators: radiation therapy for cancer, sterilization of medical supplies such as bandages, and irradiation of food to eliminate microbial contamination.



(Left) A familiar type of waveguide is optical fiber: light waves are channeled along the interior of the fiber rather than leaking out the sides. (Right) Waveguides for small accelerators, however, must be hollow to accommodate both the driving laser light and the particle beam in the same channel. They must also be optimized for electromagnetic waves with a transverse-magnetic orientation, which optical fiber is not. Shown here is a scanning electron microscope image of a 3D-printed dielectric waveguide.

forces “small” particle accelerators to be such large, cumbersome, and specialized machines. By contrast, infrared and visible-light waveguides—if they could be made to reflect TM waves—would be sized in mere microns. And infrared and visible-light lasers are not only vastly more compact than microwave sources; they are also vastly more powerful.

Mind the gap

So Simakov bucked the prevailing wisdom and set out to build an infrared-driven electron accelerator. If she could somehow invent a waveguide that reflects TM waves with a suitably slower-than-light phase velocity—well, that would be miracle number one. Miracle number two would be manufacturing waveguides and other tiny components with the tight tolerances required to

move inside conducting metals, higher-frequency light oscillates too fast for the electrons to match pace. Instead, what makes various materials reflect certain frequencies of infrared and visible light, the way a strawberry reflects red, lies in its molecular structure: the regular, repeating arrangement of atomic nuclei. The mathematical details of how this comes about are not particularly straightforward, but fundamentally, the nature and spacing of a series of tiny, distinct “cells” for electrons in the material to occupy, dictated by the repeating lattice of atomic nuclei, results in a pattern of allowed and disallowed electron energies. Allowed energy ranges, or bands, are separated by disallowed gaps.

When an electromagnetic wave strikes a material, the outcome depends on the energy of the wave, which is determined by its

To miniaturize a functional accelerator, we needed to innovate on both the waveguide and the emitter.

obtain the phase-velocity match. If she could do all that, then the whole system would be both powerful and portable. It would serve the same range of applications as current microwave-based accelerators (and perhaps many others), while being easily carried around by hand, like a briefcase.

Right away, Simakov realized that 3D printing offered a means of manufacturing the tiny waveguides. The printers have the necessary micron-scale control, and with only minor modifications, 3D-print resin would probably be a suitable dielectric. The biggest challenge, she knew, would be to engineer the structure of the 3D-printed waveguide channel to reflect TM waves with the right phase velocity. For that, she decided to go back to basics.

While slower-frequency light, such as microwaves, can be reflected by the oscillating motion of electrons that are free to

frequency. If the wave’s frequency corresponds to an energy within one of the material’s allowed energy bands, then the material can accommodate the wave passing through. If the frequency corresponds to one of the disallowed gaps, however, the wave is reflected back. Therefore, what Simakov needed to do was engineer a dielectric with some kind of regular, repeating pattern at the micron scale and adjust its pattern and spacing so that her infrared laser resides in the middle of a disallowed energy gap. Then with a little fine tuning, she could be sure to guide the waves she needs to guide: TM waves with the right phase velocity.

“We went about this by brute force,” Simakov explains. “At a scale too small to see by naked eye, our waveguides are made up of an alternating patchwork of 3D-print resin and empty space. In other words, we used precise physical gaps to make the precise energy gap.”

This approach worked wonders, with just one slight flaw: standard 3D-print resin isn't quite up to the task. In order to give the resin the right PBG attributes, its optical properties would need a slight upgrade. So Simakov worked with materials scientist Robert Gilbertson, his postdoctoral researcher Ethan Walker, and others in the Los Alamos materials science and technology division to devise a solution. They decided to create a specialized nanoparticle infusion for the resin.

The effect they were after is similar to looking at the surface of a placid lake: Look straight down, or nearly so, and you'll see what's underwater; light crosses the water-air boundary. But look farther out, and you'll see a reflection of the sky—that is, the light you see is kept on one side (the air side, in this case) of the boundary. The angle of incidence for the light striking an interface between two materials at which this shift from transmission to reflection occurs depends upon a property known as the index of refraction. For water, the index of refraction is 1.33, and for standard 3D-print resin, it's about 1.2. Simakov calculates that she needs to get the resin's index of refraction above 2, and so far, the researchers have tried an infusion of lead nanoparticles and achieved 1.98—close but no cigar. They also tried germanium nanoparticles and succeeded with 2.05, but germanium oxidizes in air and is difficult to work with, so it may be challenging to scale up the process. But Simakov believes tweaking the process for lead will ultimately work as well.

Diamond nanostructures are an accelerator scientist's best friend

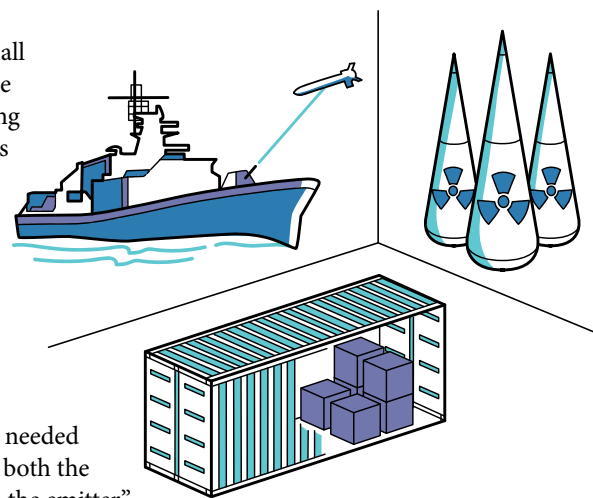
Overcoming the longstanding problem of channeling TM waves through a micron-scale waveguide is a major achievement. But that success brings with it a new challenge. A miniaturized waveguide requires a miniaturized emitter—the component that fires electrons into the waveguide.

"The wavelength of the laser determines the width of the waveguide," Simakov says. "In turn, the width of the waveguide determines the size of the emitter." Due to the electrons' mutual electrostatic repulsion, they tend to spread out in flight. In practice, this means the emitter

tip must be small enough that the beam expanding from it remains narrower than the waveguide channel when it reaches the waveguide.

"Therefore, to miniaturize a functioning accelerator, we needed to innovate on both the waveguide and the emitter."

The "we" Simakov refers to includes her Los Alamos accelerator-science colleague Heather Andrews, Simakov's postdoctoral researcher Dongsung Kim, and other colleagues from the Los Alamos accelerator operations and technology division. Together, they sought a way to produce a strong electron-emitting material that could be fashioned into an extraordinarily narrow point. They were aware of a process pioneered by researchers at Vanderbilt University, and they were able to replicate and adapt it at Los Alamos to generate crystal-perfect diamond emitters.



Some **national security applications** for compact particle accelerators using x-rays produced by electron beams: interior scans of shipping containers entering the United States, high-energy lasers to shoot down incoming missiles, and nuclear-weapons physics research, such as detonation studies at the Dual-Axis Radiographic Hydrodynamic Test facility at Los Alamos.

A nitrogen-doped diamond pyramid serves as the **emitter**. An infrared laser energizes it, causing it to launch extraordinarily narrow pulses of electrons from its nanometer-width tip. (A nanometer is a billionth of a meter.)



The virtue of using diamond is its strength. The emitter must handle a very large current density—a large number of electrons funneled through its extraordinarily narrow tip—and a weaker material would literally melt. In fact, even diamond must be upgraded to accommodate the extreme current density; it is therefore doped with nitrogen for added conductivity.

In broad strokes, the process for making the emitters works like this: Pyramid-shaped holes are etched into silicon wafers and then filled with diamond nanocrystals that grow into a single, solid structure. Then the silicon is removed to uncover a sharply pointed diamond pyramid. The pyramid tip is only nanometers in size—a thousand times narrower than the waveguide opening—as required to accommodate the widening electron beam. An

but in so doing, the laser itself loses energy. Therefore, it is important to inject additional laser light at the inlet of each waveguide. The more laser-boosted waveguides in the sequence, the greater the energy of the particles emerging in the final accelerator beam.

Spot on

Testing the electron beam a few centimeters off the cathode, Simakov produced a micron spot size with 40-kiloelectronvolt (keV)

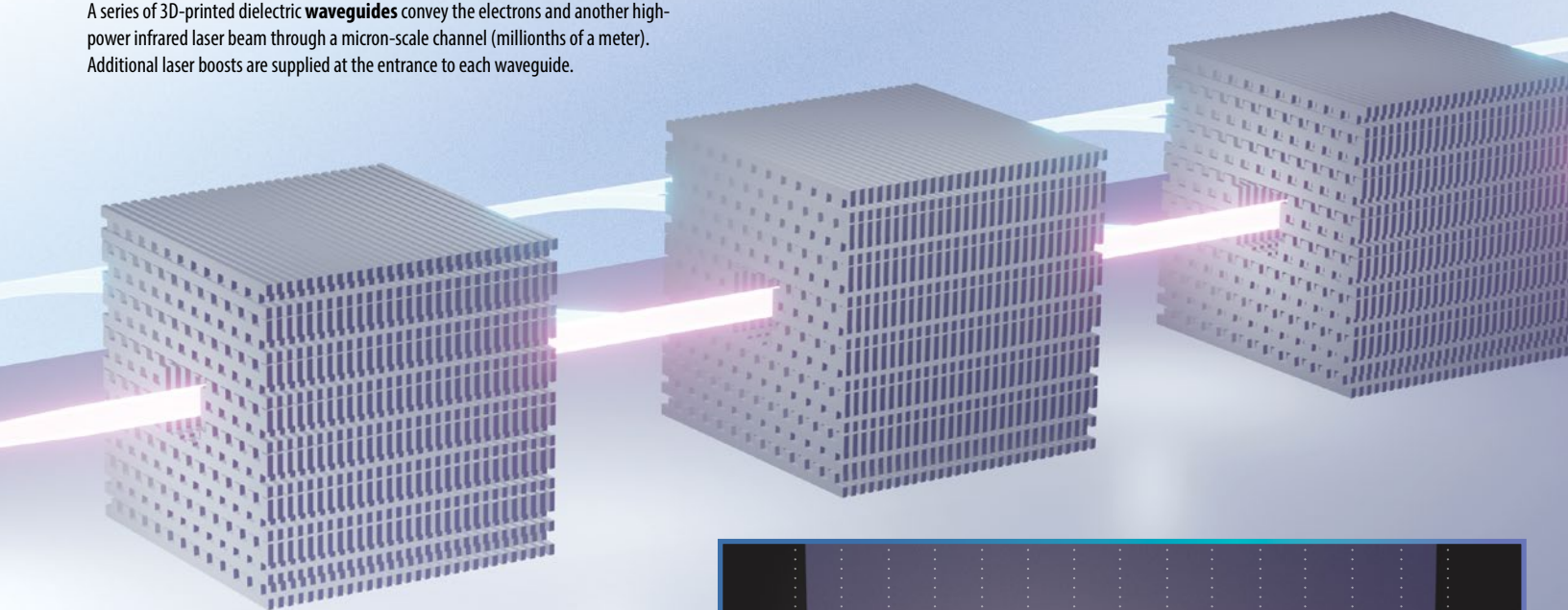
The accelerator system could easily be carried around by hand.

infrared laser, which can even be the same one that accelerates the electrons, provides the power source driving the emitter to eject electrons from its tip.

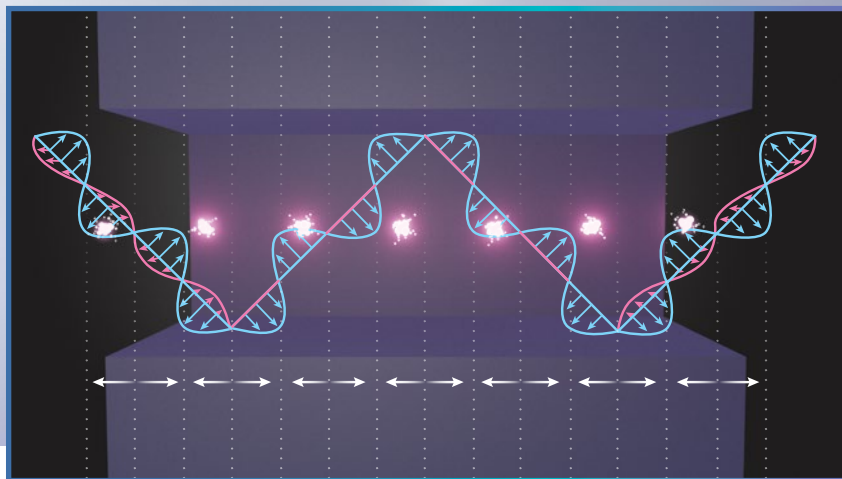
To assemble an actual accelerator system, an emitter and a series of waveguides are all aligned in a row. The acceleration occurs because the infrared laser transfers energy to the electrons,

electron energies at a beam current of 50 nanoamps, or 50 billionths of an amp. (Normally amps are used to quantify electrical current in a wire or other device; for example, half an amp flows through a 60-watt light bulb. In the context of a

A series of 3D-printed dielectric **waveguides** convey the electrons and another high-power infrared laser beam through a micron-scale channel (millionths of a meter). Additional laser boosts are supplied at the entrance to each waveguide.



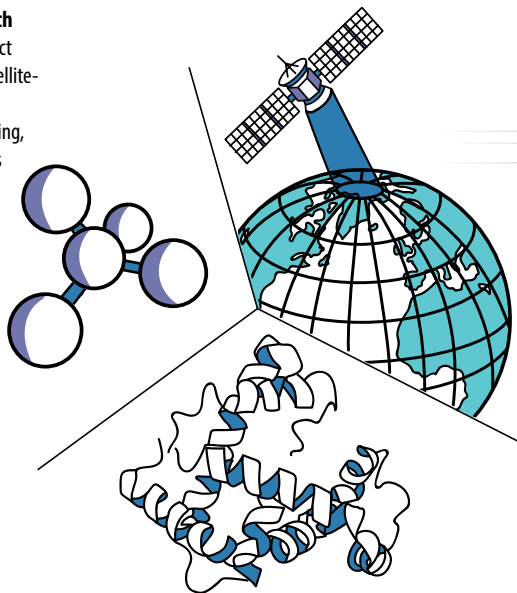
The waveguides are carefully structured to channel transverse-magnetic light waves (as shown with magnetic field component in pink). The electric field component (blue) varies diagonally as the electromagnetic wave bounces along the interior of the waveguide. Upward- and downward-directed parts of the diagonal field cancel each other out, and a net forward-backward direction remains (white arrows at bottom). Backward-directed fields push negatively charged electrons forward, and exceptionally precise timing allows electron bunches to be carried along with only that (backward-directed) component of the laser's electric field, transferring laser energy to the electrons and thereby producing the desired particle acceleration.



particle accelerator, amps quantify the rate of charged-particle flow in the beam.) In assembling a complete accelerator system, both the current and electron energy would have to increase by a factor of 20–25, to about 1 microamp and 1 megaelectronvolt (MeV), respectively, for most practical applications.

“Increasing the energy means precisely stacking a series of accelerating waveguides, and the current is limited only by desired spot size, because the more electrons you have, the more they spread out in flight,” explains Simakov. Countering that will require some additional experimentation with devices called magnetic lenses, but it should be relatively straightforward. “What’s important here is that we’ve already shown that the emitters can handle up to around 10 milliamps, which is 10,000 times more current than we really need.”

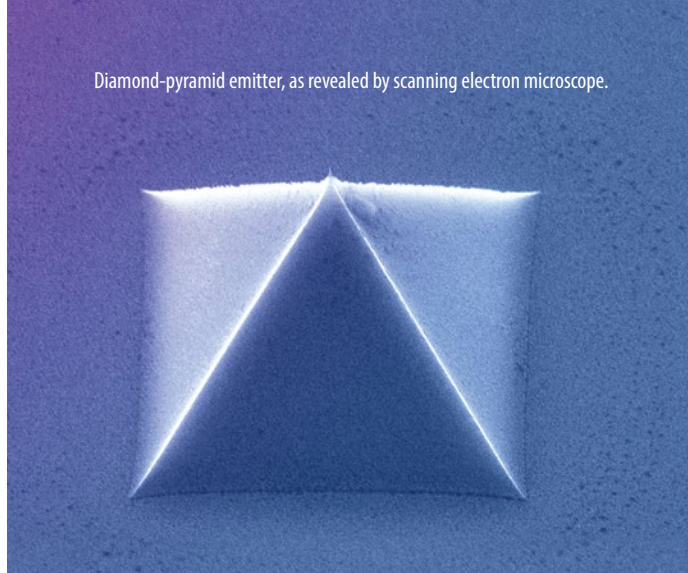
Some **scientific research applications** for compact particle accelerators: satellite-based electron beams to study auroras and lightning, x-ray free-electron lasers for molecular-level imaging, and other advanced light sources across the electromagnetic spectrum to study, for example, protein folding and enzyme activity.



In addition to seeking to tighten the focus of a beam from a single emitter, Simakov has been pursuing another approach to increase the current: simultaneously firing from a whole array of emitters and subsequently combining the beams. This approach is suitable for producing rapid-pulsing, high-energy electron beams in an alternate design known as a wakefield accelerator. Either way, the outcome is the same: compact, inexpensive particle accelerators available for widespread use.

“It’s an enabling technology that we’re pioneering here at Los Alamos,” says Simakov. Indeed, many existing

Diamond-pyramid emitter, as revealed by scanning electron microscope.



applications—particularly in the medical, research, and national security arenas—will benefit tremendously from tabletop-accelerator technology. But according to Simakov, that’s only part of the story.

*There will be
amazing applications
that don’t yet exist.*

“I think there will also be amazing applications that don’t yet exist,” she adds. “I mean, there’s never been a particle accelerator you can carry around by hand. Not even close. But every time I look at my phone—an ingenious blend of computer, wireless communication, touch screen, camera, GPS receiver, and other components—I am reminded of just how much becomes possible whenever key technologies are miniaturized.” **LDRD**

—Craig Tyler

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The radiometer suite called ICERAD (not an acronym) sits collecting data from atop an ice floe in the frigid Arctic during the 2019–2020 Multidisciplinary Drifting Observatory for the Study of Arctic Climate (MOSAic) expedition. ICERAD includes skyward-pointing radiometers to measure shortwave (visible light) and longwave (infrared) radiation, as well as temperature and humidity sensors. This instrument suite is just one of many that comprise the mobile laboratory that is operated by the Los Alamos Field Instrument Deployments and Operations (FIDO) Team. In the background, the Research Vessel *Polarstern*, home base during the year-long expedition, is invitingly aglow. For more about the FIDO team and the climate science laboratories it supports, see “To the Ends of the Earth” on page 20.

CREDIT: David Chu/LANL. Image courtesy of the U.S. Department of Energy Atmospheric Radiation Measurement (ARM) user facility.

Inset: Polar bears will occasionally approach the instruments or infrastructure on the ice floe surrounding the *Polarstern*. For the safety of the bears and the scientists alike, it’s important that the bears not become accustomed to being in camp, so the expedition’s polar bear guards use flares to safely scare the bears away.

CREDIT: Alfred Wegener Institute, Esther Horvath. Used with permission.



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About half a million human visitors—and a similar number of migrating bats—descend into Carlsbad Caverns in southeastern New Mexico each year. Statistically, however, the humans are far more likely to use the walking path and handrail (seen here in the middle of the shaft of sunlight streaking in from the cave entrance). *CREDIT: Craig Tyler/LANL*



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